UNIFORM SHEAR FLOW FAR FROM EQUILIBRIUM

By

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TABLE OF CONTENTS

ACKNOWLEDGMENTS ii

LIST OF FIGURES v

LIST OF SYMBOLS vi

ABSTRACT xi

CHAPTERS 1

1 INTRODUCTION 1

2 NONEQUILIBRIUM STATISTICAL MECHANICS 10

2.1 Formal Solution to the Liouville Equation 10
2.2 Density Fluctuations 15

3 KINETIC MODELS FOR CORRELATIONS 21

3.1 Kinetic Equations for Correlations 22
3.2 Kinetic Models for Correlations 28
3.3 Steady State Correlations 33
3.4 Examples 36
3.4.1 Equilibrium States 37
3.4.2 Stationary States Near Equilibrium 40

4 TRANSPORT EQUATIONS FOR UNIFORM SHEAR FLOW 45

4.1 Stationary State Solution 45
4.2 Normal Solution 53
4.3 Hydrodynamic Equations 58

5 TWO TIME CORRELATION EQUATION 62
5.1 Linearized Hydrodynamic Equations 63
5.2 Hydrodynamic Modes 67
6 EQUAL TIME CORRELATION FUNCTION 83
7 CONCLUSIONS 87
APPENDICES 91
A DENSITY FLUCTUATIONS 91
B DERIVATION OF KINETIC EQUATIONS 96
C DERIVATION OF KINETIC MODEL 101
D EQUILIBRIUM EXCITATION 103
E FIRST ORDER APPROXIMATION 106
F TRANSPORT COEFFICIENTS 109
G THE HYDRODYNAMIC MODES 118
H CORRELATION FUNCTIONS 121
BIBLIOGRAPHY 122
BIOGRAPHICAL SKETCH 125

LIST OF FIGURES

3.1 Real and imaginary parts of the extended hydrodynamic modes from the BGK model (in units of ν). $\pm$ indicates sound modes, H the heat mode and S the shear modes. 39

4.1 Shear viscosity $\eta(a)$(solid line) and viscometric function $\Psi(a)$ (dashed curve) are shown as function of a. η is in unit of p_s/ν, Ψ is in unit of p_s/ν^2 and a is in unit of ν. 52

4.2 The diagonal parts of the generalized thermal conductivity, $\lambda_{jj}(a)$ are shown as a function of a. The solid line is for $j = y$, the dashed line is for $j = x$, and the dash-dot line is for $j = z$. λ_{jj} is in unit of $k_B p_s/m\nu$ and a is in unit of ν. 60

5.1 Critical lines for stability are shown. The BGK-kinetic model gives the solid line and the other three lines are from Navier-Stokes order for different densities. Dashed-dot line is for $n^* = 0$, dotted curve is for $n^* = 0.2$ and dashed curve is for $n^* = 0.4$. All are in units of the mean free path and mean free time. 71

5.2 Time evolution of (a)$\delta\widetilde{u}_x(t^*)$ and (b) $\delta\widetilde{u}_y(t^*)$ for $a* = 0.5$ and $k* = 0.1$. 77

LIST OF SYMBOLS

a shear rate

$A(t)$ physical observable at time t

$A_{\alpha\beta}$ matrix

b_{ij} scattering operator

$B_{\alpha\beta}$ matrix

$B(t)$ physical observable at time t

c sound velocity

C correlation function at two phase points and times

$\tilde{C}$ Fourier representation of C

C_v specific heat

$C_{\alpha\beta}$ hydrodynamic correlation function

$C_{\alpha\beta}$ matrix

$D_{\alpha\beta}$ matrix

D_T thermal diffusivity

$f^{(s)}$ s-particle reduced distribution function

$\hat{f}^{(s)}$ s-particle microscopic phase density

f solution to the Boltzmann equation

$\tilde{f}$ Fourier representation of f

f_s stationary solution to the Boltzmann equation

f_ℓ local equilibrium distribution function

f_e Maxwell-Boltzmann distribution function

$F_{\alpha\beta}$ matrix

g_α eigenfunctions of inhomogeneous linearized Boltzmann operator

g_i velocity functions in Appendix E

G single time pair correlation function

$G_{\alpha\beta}$ hydrodynamic pair correlation function

G_{11} density fluctuation

H^{ij} matrix

h_α complex conjugates of g_α

h_α integral function in Appendix E

I linearized Boltzmann collision operator

$I_{\alpha\beta}$ matrix

J Boltzmann collision operator

k wavevector

K Green's function

$K_{\alpha\beta}$ matrix

k_B Boltzmann constant

l_{mfp} mean free path

L Liouville operator

L velocity operator from chapter 4

$\mathcal{L}$ inhomogeneous linear operator

$\tilde{\mathcal{L}}$ Fourier representation of $\mathcal{L}$

m mass of the particle

n density

$N_{\alpha\beta}$ matrix

p pressure

p_o equilibrium pressure

P projection operator

$\mathbf{q}$ heat flux

Q constant

R resolvent function

s_i eigenvalues of the matrix F

S dynamic structure factor

t time

t_{ij} monentum flux, pressure tensor

T_{ij} volume integral of t_{ij}

T temperature

$T(1,2)$ binary scattering operator

$\mathbf{u}$ flow velocity

$\mathbf{v}$ velocity variable

$\mathbf{v}'$ velocity variable relative to the uniform shear flow velocity

v_o thermal velocity

$\mathbf{V}$ peculiar velocity

$V(r)$ potential energy

w inhomogeneous term in the temperature equation

x dimensionless variable

$X_{\alpha,i}$ coefficients of the hydrodynamic gradients

$Y_{\alpha,i}$ coefficients of the hydrodynamic gradients

y_α hydrodynamic variables

z roots of a determinant equation

Z complex probability integral

α dimensionless parameter

β inverse temperature multiplied to k_B^{-1}

Γ sound damping constant

γ source to the pair correlation function G

γ_{lk}^{ij} transport coefficients

ϵ energy density in Chapter 2

ϵ universal parameter

$\zeta^{(i)}$ eigenvectors of the matrix F

$\eta^{(j)}$ biorthogonal set of $\zeta^{(i)}$

η shear viscosity

η_B shear viscosity from the Boltzmann equation for hard spheres

θ dimensionless parameter

κ thermal conductivity

κ_B thermal conductivity from the Boltzmann equation for hard spheres

Λ linear operator

λ proportional constant in the external force

λ_α eigenvalues of $\mathcal{L}$

λ_{jj} diagonal parts of generalized thermal conductivity

μ bulk viscosity

ν collision frequency

$\xi^i_{\alpha,j}$ transport coefficients

ρ mass density

$\rho(t)$ $N-$body distribution function

ρ_ℓ local equilibrium distribution function

σ diameter of the hard sphere

ϕ_α linear combination of the summational invariants

χ equilibrium pair correlation function

ψ_α summational invariants

Ψ_i viscometric functions

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UNIFORM SHEAR FLOW FAR FROM EQUILIBRIUM

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Nonequilibrium phenomena are well understood for states near equilibrium. However, even the qualitative properties of transport and fluctuations far from equilibrium are poorly understood due to the complexity of the physical states. The objective here is to explore in detail dynamical properties of a simple fluid far from equilibrium for the specific case of uniform shear flow. The analysis is limited to conditions of low density for which there is a controlled kinetic theory description based in the principles of nonequilibrium statistical mechanics. These kinetic equations provide a description of both transport and fluctuations in general nonequilibrium states. However it is very difficult to solve these equations. To make this description practical far from equilibrium, a related set of model kinetic equations is constructed by retaining the essential mathematical and physical properties of the original kinetic equations, while admitting more

practical analysis. These model equations are solved for the reference state of uniform shear flow, fluctuations about that state, and for the dynamics of small perturbations from that state. In this shear flow, the shear rate is the only control parameter that measures how far the system is from equilibrium. First, the distribution function for the reference state is calculated exactly and an expansion in small spatial deviations from the reference state is performed to describe the dynamics of states near uniform shear flow. This solution to the kinetic equation also provides a hydrodynamic description, and a closed set of generalized hydrodynamic equations is derived. The associated nonlinear transport coefficients are identified and calculated for an arbitrary shear rate. The hydrodynamic modes defined by the linearized hydrodynamic equations are studied to determine the shear rate dependence of relaxation back to the reference state. A new long wavelength instability for uniform shear flow is found such that the hydrodynamic modes are growing initially for finite shear rate and sufficiently long wavelength. Finally, spatially long ranged correlations within the uniform shear state are studied at large shear rates.

CHAPTER 1
INTRODUCTION

The world in which we live consists of a large number of particles which interact in a very complex way. Statistical mechanics is the field of describing static and dynamical processes of many body systems, using probabilistic concepts. The state is specified not by the position and momenta of individual particles (it is not wrong, only impractical), but by a distribution function, $\rho(t)$, which is a probability density of the system in the N-particle phase space. The dynamics of this distribution function is calculated from the Liouville equation. With the knowledge of this function, the average value of any dynamical variable (physical observable) can be obtained in principle. However, these average values are not meaningful for describing the system unless the fluctuations about the average and actual values are known. These fluctuations also are related closely to a number of experimental methods used to probe many body systems (e.g. elastic and inelastic scattering of particles and radiation). Therefore, fluctuations are very important properties to understand. The most general type of average and the fluctuations are defined by

$$\langle A(t)\rangle_{t_0} = \int d\Gamma A(\Gamma, t)\rho(\Gamma, t_0), \tag{1.1}$$

$$(\delta A(t)\delta B(t'))_{t_0} = \int d\Gamma \delta A(\Gamma, t)\delta B(\Gamma, t')\rho(\Gamma, t_0), \tag{1.2}$$

where $A(t)$, $B(t')$ correspond to physical observables of interest at times t and t', and the bracket means the average over the distribution function at time t_0 when the system is prepared. Also, Γ denotes a point in the N-particle phase space, representing the positions and momenta of all particles, and $\delta A(t)$ means $A(t) - \langle A(t) \rangle_{t_0}$.

At equilibrium, the properties of the average values and their fluctuations are well understood, and extensive methods exist for their calculations and measurement. For instance, the averages provide the thermodynamic variables (e.g. internal energy), while the susceptibilities are related to fluctuations at equal times (e.g. specific heat). Both of these can be calculated as averages over the known Gibbs distribution function using Eqs.(1.1) and (1.2). The dynamics of fluctuations at different times in the equilibrium state also is important since it describes the linear response of an equilibrium system to small initial or external perturbations [1]. These fluctuations also are well studied both theoretically and experimentally.

In nonequilibrium states, the methods for obtaining the values of the physical observables and their fluctuations (both static and dynamic) are still in the process of developing. Significant progress has been made for states near equilibrium. For example, kinetic and hydrodynamic equations are accurate and practical for calculating average properties near equilibrium. Furthermore, the dynamics of fluctuations in states near equilibrium has been studied recently in some detail [2]. These studies show interesting qualitative differences from the corresponding fluctuations at equilibrium, such as long ranged spatial correlations [3].

Recent accurate light scattering experiments [4] support these theoretical predictions. Also, these studies have provided a simple phenomenological description, e.g. fluctuating hydrodynamics [5], to understand the mechanisms responsible for these correlations. However, for the states far from equilibrium, technical difficulties prohibit having any significant qualitative and quantitative knowledge of either average values or their fluctuations in general. The purpose of the work in this thesis is to choose a special state far from equilibrium and to explore all possible aspects of static and dynamic fluctuations presently unknown. Progress on this difficult problem has been possible because there is a well-developed kinetic theory at low density and in principle those kinetic equations are solvable for any nonequilibrium state. However their application is limited for practical purposes. In this thesis, "model" kinetic equations are developed for static and dynamic correlation functions by using fundamental functional relationships between the related kinetic equations for transport and fluctuations. These equations provide a practical basis for describing phenomena in general nonequilibrium states. To illustrate the practicality of these kinetic equations, we choose uniform shear flow state as a prototype nonequilibrium test case. The uniform shear flow state is characterized by a very simple macroscopic state. This flow is defined by a linear velocity profile along the x-axis with a constant velocity gradient along the y-axis, and constant density and temperature,

$$u_i = a_{ij} r_j, \;\; a_{ij} \equiv a\, \delta_{ix}\delta_{jy}, \;\; n = \text{constant}, \;\; T = T(t). \tag{1.3}$$

where $\mathbf{u}, n, T$ are flow velocity, density, temperature respectively. The velocity

gradient or shear rate, a, is constant and represents the single control parameter measuring how far the system is from equilibrium. If we perform local Galilean transformations $\mathbf{r}' = \mathbf{r} - \mathbf{u}(\mathbf{r})t$, $\mathbf{v}' = \mathbf{v} - \mathbf{u}(\mathbf{r})$, the macroscopic state can be transformed into the uniform local rest state. Because of this property, uniform shear flow can be generated easily with Lees-Edwards boundary conditions [6] which are simple periodic boundary conditions in the local rest frame. Also, the shear effects in uniform shear flow induce viscous heating and cause the temperature to increase in time. This heating problem can be avoided by introducing a thermostat such that the state becomes stationary. Because of this stationarity, simplicity of the macroscopic state, and the ideal boundary conditions, this state has been used as a prototype for the studies of properties in nonequilibrium systems. There have been many computer simulations [6–11] for transport properties for this state. However, theoretical studies have been restricted primarily to the limit of small shear rate [2, 12–17]. In this thesis, we explore properties such as nonlinear transport and fluctuations for states far from equilibrium for uniform shear flow and states near the uniform shear flow.

Traditionally there are two ways to calculate transport properties and fluctuations in nonequilibrium states. The first is a direct statistical mechanics approach. In this method, a formally exact solution to the Liouville equation is constructed. Use of this solution in (1.1) and (1.2) gives an explicit representation of the physical observables and their fluctuations. Generally, however, it is very difficult to obtain this solution in a practical form. Instead, a perturbation method can be used if the state is not far from equilibrium to construct an explicit form for ρ

as a small deviation from the Gibbs distribution. In Chapter 2, the correlation function near the equilibrium state is represented in this way for uniform shear flow. The resulting form is suitable for study via standard equilibrium molecular simulation, but still difficult to calculate theoretically. However at low density, it is shown that the calculation is tractable and the nonequilibrium density fluctuations are calculated as an illustration. The result shows the spatially long range correlations mentioned above, in agreement with previous phenomenological calculations [18]. This brief analysis is presented to demonstrate the new effects that occur for nonequilibrium fluctuations and to show the practical limitations of the direct computational approach for states far from equilibrium.

The second method to describe transport and fluctuations is by the kinetic theory. It is this method that is used in the remainder of the thesis. The average of any physical observable that is represented by a sum of single particle functions may be obtained as an integral over the solution to the single particle kinetic equation, $f^{(1)}$,

$$\langle A(t)\rangle_{t_0} = \int dx f^{(1)}(x,t_0)a(x,t); \quad A(t) \equiv \sum_{i=1}^{N} a_i(x,t). \tag{1.4}$$

Traditional kinetic theory provides an equation for the single particle reduced distribution function derived from an approximation to the BBGKY hierarchy. At low density, the relevant approximation leads to the famous Boltzmann equation. Closely related kinetic equations for fluctuations also can be constructed by applying the same many body analysis used to derive the Boltzmann equation [19]. Generally, these kinetic equations are very difficult to solve except for

a few special cases, or for states near equilibrium. Sophisticated Monte Carlo simulation methods are available to solve the Boltzmann equation [20], but they have not been adapted to solve the equations for fluctuations. Exact solutions to the Boltzmann equation far from equilibrium are still very few. A formal solution exists for uniform shear flow [21, 22], but this solution provides only equations for moments of the distribution function rather than for the distribution function itself. In the case of the Boltzmann equation, these difficulties have been circumvented by replacing the collision operator with a simpler form. The result is a "model" kinetic equation that preserves the most important mathematical and physical properties of the Boltzmann equation, while allowing more practical analysis. The choice considered here is the well known BGK model [23]. Exact solutions to the BGK-Boltzmann equation have been obtained for several cases [24] including uniform shear flow [25]. Also, the BGK model has been proved to provide an accurate representation of the Boltzmann equation for uniform shear flow [26]. A primary new result of this thesis is the development of a corresponding kinetic model for the equations describing fluctuations. The result is then a more practical coupled set of equations for all properties of interest in general nonequilibrium states. Here, they are applied to the uniform shear flow state and the model equations are solved for arbitrary shear rates.

This kinetic description of fluctuations and transport properties is at the detailed level of the single particle phase space (position and velocity). However, it incorporates as well a "hydrodynamic" description for large space and time scales. If we are interested in space and time scales which are large compared to the mean

free path and mean free time (distance and time between collisions), it is possible that the system can be described in terms of few physical observables, the local conserved densities (mass, energy and momentum density). The averages of these local densities are called hydrodynamic variables. A closed dynamics for the hydrodynamic variables can be obtained from integration of the Boltzmann equation multiplied by the corresponding single particle functions $(1, \mathbf{v}, v^2)$. The hydrodynamic equations can be linearized around the reference state to determine the hydrodynamic modes (excitations) which describe the response of the state to the small perturbations. In Chapters 4, 5 and 6, this hydrodynamic description is constructed for states far from equilibrium. First, the distribution function at and near the reference state of uniform shear flow is calculated for arbitrary shear rate. This solution then is used to derive a closed set of generalized nonlinear hydrodynamic equations. This gives a complete description of all average properties of interest. A nonequilibrium fluctuation-dissipation relation is used to express the dynamics of fluctuations of the hydrodynamic variables in terms of the hydrodynamic modes. For mode excitations near the uniform shear state, a long wavelength instability is found such that at any finite value of the shear rate, modes of sufficiently long wavelength exhibit initial growth rather than relaxation. Finally, long range spatial correlations at large shear rates are investigated by calculating the density fluctuations using these same hydrodynamic modes. However there is a limitation on the length scale for studying spatial correlations because of the long wavelength instability.

The presentation of this thesis is organized as follows. In Chapter 2, the exact formal solution to the Liouville equation for uniform shear flow is derived. To illustrate an application, the density fluctuations are calculated in detail for a low density gas at small shear rate. The difficulties of applying this approach at large shear rate are noted. In Chapter 3, the kinetic theory for transport and fluctuations at low density is recalled, and three equations for corresponding kinetic models are constructed. The formal solutions to these model equations are obtained. To illustrate the practicality of the kinetic model, two examples are discussed. In the remaining chapters, the three kinetic model equations are specialized to the case of uniform shear flow. In Chapter 4, the stationary solution, f_s, is determined exactly for all shear rates and then a special "normal" solution near the stationary state is constructed. The normal solution allows calculation of the heat and momentum fluxes in terms of the hydrodynamic gradients and identification of the hydrodynamic equations. The transport coefficients also are calculated in detail from the normal solution. These fluxes and new transport coefficients describe transport properties far beyond the usual Navier-Stokes order (e.g. they describe strong rheological effects). In Chapter 5, two time correlation functions are examined. These functions represent the linear response to a small perturbation of uniform shear flow. With these functions, both the modes of relaxation and the stability of uniform shear flow are analyzed. The dispersion relations are solved to determine these modes as a function of the shear rate. A new long wavelength instability of the uniform shear flow state is found. This instability is compared with computer simulation results, showing an excellent

agreement between theory and simulation during the initial stages. In Chapter 6, equal time correlation functions are studied. The long range spatial correlations in the density fluctuations are investigated again, now at large shear rates. An algebraic decay is expected from earlier calculations based on small shear rate, due to coupling of the hydrodynamic modes at equilibrium. These results are extended to large shear rate using the generalized hydrodynamic modes of Chapter 5. The results are summarized in Chapter 7, and topics for further study are discussed.

CHAPTER 2
NONEQUILIBRIUM STATISTICAL MECHANICS

In this chapter, a formal solution to the Liouville equation with a nonconservative force is derived for uniform shear flow. The solution to this equation is used to calculate fluctuations in this nonequilibrium state. To illustrate its practical application, the density fluctuations are computed at low density and small shear rate.

2.1 Formal Solution to the Liouville Equation

In statistical mechanics, the state of the system at time t is described by the N-body distribution function, $\rho(x_1, \cdots, x_N, t)$. Here $x_i \equiv (\mathbf{q}_i, \mathbf{p}_i)$ and $\mathbf{q}$, $\mathbf{p}$ are the coordinates and momenta of the particles in phase space, respectively. The time dependence of the function is determined from the Liouville equation. The system to be described is in contact with external reservoirs and the associated interaction between the system and the reservoirs will be represented by nonconservative forces. The Liouville equation with the external force is

$$\left(\frac{\partial}{\partial t} + L + \Delta\right)\rho = 0, \tag{2.1}$$

where

$$L \equiv \sum_{\alpha=1}^{N} \left(\frac{\mathbf{p}_\alpha}{m} \cdot \nabla_{\mathbf{q}_\alpha} + \mathbf{F}_{ext}(\mathbf{p}_\alpha) \cdot \nabla_{\mathbf{p}_\alpha} \right) + \frac{1}{2} \sum_{\alpha \neq \beta} \mathbf{F}(\mathbf{q}_\alpha - \mathbf{q}_\beta) \cdot \nabla_{\mathbf{p}_\alpha}, \tag{2.2}$$

$$\triangle \equiv \sum_{\alpha} \nabla_{\mathbf{p}_\alpha} \cdot \mathbf{F}_{ext}. \tag{2.3}$$

The $\mathbf{F}_{ext}$ is an external force and $\mathbf{F}$ represents the interaction between particles. By solving this equation, physical observables of interest and their fluctuations can be calculated using Eqs.(1.1) and (1.2). Here, we look for the solution corresponding to uniform shear flow. This flow is generated by Lees-Edwards boundary conditions [6]. These conditions are the usual periodic boundary conditions along the x and z axes, but with shearing conditions at $y = \pm L$,

$$\begin{aligned} p_x(y = -L) &= p_x(y = L) - 2mu_x(y = L), \\ q_x(y = -L) &= q_x(y = L) - 2u_x(y = L)t. \end{aligned} \tag{2.4}$$

These are not the usual local boundary conditions where a particle's velocity accommodates locally the velocity of the wall. Instead these are nonlocal relations between particles leaving at $y = L$ and those entering at $y = -L$. To motivate this, it is useful to make a Galilean transformation to the local Lagrangian frame determined by the macroscopic flow velocity $u_i = a_{ij} r_j$,

$$\begin{aligned} \tilde{p}_{\alpha,i} &= p_{\alpha,i} - mu_i, \\ \tilde{q}_{\alpha,i} &= q_{\alpha,i} - u_i t, \end{aligned} \tag{2.5}$$

where i, j denotes a Cartesian coordinate. Then it is seen that the boundary conditions (2.4) become simple periodic boundary conditions. This is particularly useful for molecular dynamics simulations of uniform shear flow.

It is convenient to represent the Liouville operator in the mixed set of variables, $\{\mathbf{q}_\alpha, \tilde{\mathbf{p}}_\alpha\}$. Then the new Liouville operator $\tilde{L}$ becomes

$$\tilde{L} = \sum_{\alpha=1}^{N} \frac{\tilde{p}_{\alpha,i}}{m} \frac{\partial}{\partial q_{\alpha,i}} + a_{ij} \left(q_{\alpha,j} \frac{\partial}{\partial q_{\alpha i}} - \tilde{p}_{\alpha j} \frac{\partial}{\partial \tilde{p}_{\alpha i}} \right) + F_{ext,i}(\tilde{\mathbf{p}}_\alpha) \frac{\partial}{\partial \tilde{p}_{\alpha,i}} + \frac{1}{2} \sum_{\alpha \neq \beta} F_i(\mathbf{q}_\alpha - \mathbf{q}_\beta) \frac{\partial}{\partial \tilde{p}_{\alpha,i}}, \tag{2.6}$$

$$\widetilde{\Delta} = \sum_{\alpha} \frac{\partial}{\partial \tilde{p}_{\alpha,i}} F_{ext,i}(\tilde{\mathbf{p}}_\alpha). \tag{2.7}$$

We look for solutions of the form

$$\rho = \rho(\{\tilde{\mathbf{p}}_\alpha\}, \{\mathbf{q}_\alpha - \mathbf{q}_\beta\}, t), \tag{2.8}$$

which expresses translational invariance at fixed $\{\tilde{p}_\alpha\}$. This is sufficient to assure that the macroscopic state is indeed that of uniform shear flow. It is convenient to represent the solution in terms of the deviation from the local equilibrium distribution function, ρ_ℓ, so we define a new phase function, D,

$$\rho(\tilde{\Gamma}, t) = \rho_\ell(\tilde{\Gamma}, t) \mathrm{e}^{D(\tilde{\Gamma}, t)}, \tag{2.9}$$

where $\tilde{\Gamma}$ is a phase coordinate $\{\mathbf{q}_\alpha, \tilde{\mathbf{p}}_\alpha\}$, and ρ_ℓ is a local equilibrium distribution function, $\rho_\ell = \exp[-(q(t) - \beta(t)\widetilde{H})]$. The $q(t)$ is a normalization factor, $\beta = 1/k_B T(t)$, and $\widetilde{H} = \sum_\alpha \frac{\tilde{p}_\alpha^2}{2m} + \frac{1}{2} \sum_{\alpha \neq \beta} V(q_{\alpha\beta})$, where V represents an

interaction potential between two particles. and $q_{\alpha\beta}$ denotes the distance between two particles α and β. Substitution of this expression (2.9) into the Liouville equation gives the equation for $D(t)$.

$$\left(\frac{\partial}{\partial t}+\tilde{L}\right) D(t) = -\widetilde{\Delta} - \left(\frac{\partial}{\partial t}+\tilde{L}\right) \log f_\ell \tag{2.10}$$

$$= -\widetilde{\Delta} - f_\ell \frac{\partial \beta}{\partial t}(\langle \widetilde{H}\rangle_\ell - \widetilde{H}) + \beta \tilde{L}\widetilde{H} f_\ell. \tag{2.11}$$

The general solution, $D(t)$, is

$$D(t) = e^{-t\tilde{L}} D(t=0) - \int_0^t d\tau e^{-(t-\tau)\tilde{L}} \left[\widetilde{\Delta} + \frac{\partial \beta(\tau)}{\partial \tau}(\langle \widetilde{H}\rangle_\ell - \widetilde{H}) - \beta(\tau)\tilde{L}\widetilde{H}\right]. \tag{2.12}$$

The time dependence in the brackets on the right side occurs entirely through the temperature $T(t)$. Therefore, at long times, a stationary state is possible if we choose the external force to hold the temperature constant. The nonconservative force can be fixed as being proportional to the velocity relative to local flow velocity,

$$\mathbf{F}_{ext}(\tilde{\mathbf{p}}_\alpha) = -\lambda \tilde{\mathbf{p}}_\alpha, \tag{2.13}$$

where the constant λ can be determined by requiring stationarity. Since the only time dependence comes from temperature, we need to find the time dependent average energy equation. The microscopic energy density is defined by

$$\tilde{\epsilon} = \sum_\alpha \frac{\tilde{p}_\alpha^2}{2m}\delta(\mathbf{r}-\mathbf{q}_\alpha) + \frac{1}{2}\sum_{\alpha\neq\beta} V(q_{\alpha\beta})\delta(\mathbf{r}-\mathbf{q}_\alpha). \tag{2.14}$$

The average energy equation can be obtained by the integration of the Liouville

equation with the energy density,

$$\int d\tilde{\Gamma}\,\tilde{\epsilon}\,\langle\frac{\partial}{\partial t}+\tilde{L}+\widetilde{\Delta}\rangle\,\tilde{\rho}=0. \tag{2.15}$$

By using the translational invariant property, the average energy equation can be written as

$$\frac{\partial}{\partial t}\langle\tilde{\epsilon}\rangle_t=-a_{ij}\langle\tilde{t}^K_{ij}\rangle_t+\langle\sum_\alpha \mathbf{F}_{ext}(\tilde{\mathbf{p}}_\alpha)\cdot\tilde{\mathbf{p}}_\alpha\rangle_t, \tag{2.16}$$

where $\langle\cdots\rangle_t$ means average over $\rho(t)$ like in $\langle 1.1\rangle$, and $\tilde{t}^K_{ij}=\sum_\alpha \frac{\tilde{p}_{\alpha i}\tilde{p}_{\alpha j}}{m}\delta(\mathbf{r}-\mathbf{q}_\alpha)$. Because of the translational invariance, the potential part of momentum flux does not contribute to the energy equation for uniform shear flow. Now the stationary condition is imposed on Eq.$\langle 2.16\ \rangle$ as $\frac{\partial}{\partial t}\langle\tilde{\epsilon}\rangle_t=0$. The proportionality constant λ is obtained as

$$\lambda=-\frac{a_{ij}\langle\tilde{T}^K_{ij}\rangle}{\langle 2\widetilde{K}\rangle}, \tag{2.17}$$

where $\tilde{T}^K_{ij}$ is a volume integral of $\tilde{t}^K_{ij}$ and $\widetilde{K}$ is a kinetic energy,

$$\tilde{T}^K_{ij}=\sum_\alpha\frac{\tilde{p}_{\alpha i}\tilde{p}_{\alpha j}}{m}, \tag{2.18}$$

$$\widetilde{K}=\sum_\alpha\frac{\tilde{p}^2_\alpha}{2m}. \tag{2.19}$$

Then $D(t)$ from $\langle 2.12\rangle$ can be stationary by taking the infinite time limit,

$$D_s(\tilde{\Gamma})=-\int_0^\infty d\tau\, e^{-\tau\tilde{L}}\left[\beta a_{ij}\tilde{T}_{ij}-\beta\frac{a_{ij}\langle\tilde{T}^K_{ij}\rangle}{\langle\widetilde{K}\rangle}\langle\widetilde{K}-\langle\widetilde{K}\rangle\rangle\right], \tag{2.20}$$

where "s" means stationary and $\tilde{T}_{ij}$ is total momentum flux, $\tilde{T}_{ij}=\sum_\alpha\frac{\tilde{p}_{\alpha i}\tilde{p}_{\alpha j}}{m}+$

$\frac{1}{2}\sum_{\alpha\neq\beta}(q_{\beta i}-q_{\alpha i})\frac{\partial V(q_{\alpha\beta})}{\partial q_{\alpha j}}$. This D_s gives a formal stationary solution to the Liouville equation for uniform shear flow,

$$\rho_s = \rho_e e^{D_s}, \tag{2.21}$$

where ρ_e is an equilibrium distribution function. By using this stationary solution, it is possible to calculate the average of the physical variables and their fluctuations from Eqs.(1.1) and (1.2) in principle. As an illustration, in the next section we will discuss the equal time density fluctuations.

2.2 Density Fluctuations

In the last section, we constructed the formal solution to the Liouville equation for uniform shear flow. With this solution, in this section, we will calculate the equal time density fluctuation. This fluctuation can be written by using Eq.(1.2) and the related physical variable, density, $n = \sum_\alpha \delta(\mathbf{q}_\alpha - \mathbf{r})$. Then the density fluctuation can be represented in terms of the correlation function,

$$\langle \delta n(\mathbf{r})\delta n(\mathbf{r}')\rangle_{ne}, \tag{2.22}$$

where $\langle\cdots\rangle_{ne}$ denotes average over the stationary nonequilibrium distribution function, ρ_s. This representation is sometimes called density correlation functions and it has the same meaning as density fluctuations. These density correlation functions can be rewritten in terms of the phase function D_s by using the $\rho_s =$

$\rho_e e^{D_s}$ (2.21),

$$(\delta n(\mathbf{r})\delta n(\mathbf{r}'))_{ne} = (\delta n(\mathbf{r})\delta n(\mathbf{r}')e^{D_s})_e, \tag{2.23}$$

where $(\cdots)_e$ means average over the equilibrium distribution function, ρ_e, and actually it is the Gibbs distribution function. Now the density fluctuations are expressed in terms of three phase functions, averaged over the equilibrium distribution. This representation is suitable for standard equilibrium molecular dynamics simulations, because the equilibrium distribution is well known. However, it is not practical for theoretical calculations except for states near equilibrium, since the factor e^{D_s} is very complicated.

For states near equilibrium (for small a), a perturbation method can be applied to the solutions (2.20) and (2.21). Then, the first term in (2.20) will be dominant (the second term is proportional to a^2), and the distribution function can be written as

$$\rho_s = \rho_{s\ell}(1 - \beta\, a \int_0^\infty d\tau\, \tilde{T}_{xy}(\tau)), \tag{2.24}$$

where $\tilde{T}_{xy}(\tau) \equiv e^{-\tau\tilde{L}}\tilde{T}_{xy}$. For states near equilibrium, the density fluctuations are

$$(\delta n(\mathbf{r})\delta n(\mathbf{r}'))_{ne} = (\delta n(\mathbf{r})\delta n(\mathbf{r}'))_e - \beta\, a \int_0^\infty d\tau (\delta n(\mathbf{r})\delta n(\mathbf{r}')\tilde{T}_{xy}(\tau))_e. \tag{2.25}$$

The first term represents an equilibrium density fluctuation and is usually written as

$$(\delta n(\mathbf{r})\delta n(\mathbf{r}'))_e = n\delta(\mathbf{r} - \mathbf{r}') + n^2[g(r) - 1], \tag{2.26}$$

where n is the average density at equilibrium and $g(r)$ is the pair correlation

function. At low density, the second term can be neglected, so the density fluctuations at equilibrium have spatially very short range correlations. The second term of Eq.(2.25) involves three phase functions and is represented with a time integral which is similar to the Green-Kubo formula. The Green-Kubo formula is involved with time integration of the flux-flux time dependent correlation function and gives a related transport coefficient, while our second term has a time integral of two density fluctuations at one time and a flux at the other time correlation and it gives a stationary nonequilibrium density fluctuation. We can see from this representation that the dynamical origin is very important for determining a new effect of the stationary nonequilibrium fluctuation. This point will be more clear if the second term of (2.25) is written without time integration. It is possible to do so by using the relationship

$$T_{ij}(t) = \frac{\partial}{\partial t} M_{ij}(t), \quad M_{ij}(t) \equiv \sum_{\alpha} q_{\alpha,j}(t) p_{\alpha,i}(t). \tag{2.27}$$

Then the density fluctuation for uniform shear flow is written as

$$\langle \delta n(\mathbf{r}) \delta n(\mathbf{r}') \rangle_{ne} = \langle \delta n(\mathbf{r}) \delta n(\mathbf{r}') \rangle_{e} - \beta a \lim_{t \to \infty} \langle \delta n(\mathbf{r}) \delta n(\mathbf{r}') [\widetilde{M}_{xy}(t) - \widetilde{M}_{xy}(0)] \rangle_{e}. \tag{2.28}$$

From this expression, it is clearly seen that equilibrium "time dependent" fluctuations are the origin of the effect of the nonequilibrium steady correlation such as spatial long range correlations.

Even though the formal representation is given for density fluctuation like (2.28), it is very hard to solve analytically because of the time dependence which comes from the formal Liouville operator. However, at low density, the well developed kinetic theory is available to calculate the density fluctuations. Here we will use the recipe from the paper by Dufty [27] and Groome, Gubbins and Dufty [28] to calculate the density fluctuation without detailed explanations. At low density, the time dependent correlation can be represented as

$$\langle \delta n(\mathbf{r}) \delta n(\mathbf{r}') \widetilde{M}_{xy}(t) \rangle_e = \int d\mathbf{q} d\mathbf{p}\, f_0\, p_x\, q_y\, T_t \{ \delta(\mathbf{r}-\mathbf{q}) \delta(\mathbf{r}'-\mathbf{q}') \} - \int_0^t d\tau \int d\mathbf{q} d\mathbf{p}\, f_0\, p_x\, q_y\, T_{t-\tau}\, n J_s [T_\tau \delta(\mathbf{r}-\mathbf{q}), T_\tau \delta(\mathbf{r}'-\mathbf{q}')], \tag{2.29}$$

where now T_t depends on the inhomogeneous linearized Boltzmann collision operator instead of a formal Liouville operator,

$$T_t = \exp -(\mathbf{v} \cdot \nabla + nI)t. \tag{2.30}$$

The J is a Boltzmann collision operator

$$J[f,g] = \int d\mathbf{v}_1 (\mathbf{v}-\mathbf{v}_1) b\, db\, d\varphi [f'(v) g'(v_1) - f(v) g(v_1)], \tag{2.31}$$

and the prime denotes the stage after collisions. The I is a linearized Boltzmann operator,

$$nIX = \int d\mathbf{v}_1 (\mathbf{v}-\mathbf{v}_1) b\, db\, d\varphi f_0(v_1) [X(v) + X(v_1) - X'(v) - X'(v_1)], \tag{2.32}$$

and $f_0(v_1)$ is a Maxwell-Boltzmann distribution function. Also J_s has the symmetrized form

$$J_s[f,g] = J[f,g] + J[g,f]. \tag{2.33}$$

The calculation of (2.29) will be simpler if the arguments in the Boltzmann collision operator J_s are represented in Fourier space. Then, after a few steps of calculations, (2.29) becomes

$$\begin{aligned}
&\langle \delta n(\mathbf{r})\delta n(\mathbf{r}')\widetilde{M}_{xy}(t)\rangle_e = \\
&-\frac{1}{(2\pi)^3}\int d\mathbf{k}\, i\frac{\partial}{\partial k_y} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\int_0^t d\tau\ (p_x,\ nJ_s[\tilde{a}(\mathbf{k},\mathbf{v}),\tilde{a}(-\mathbf{k},\mathbf{v})]) \\
&-\frac{1}{(2\pi)^3}\int d\mathbf{k}\, e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\int_0^t d\tau\ \left(I^{-1}(1-e^{-(t-\tau)nI})\frac{v_x v_y}{m}, J_s[\tilde{a}(\mathbf{k},\mathbf{v}),\tilde{a}(-\mathbf{k},\mathbf{v})]\right),
\end{aligned} \tag{2.34}$$

where (X,Y) defined by

$$(X,Y) = \int d\mathbf{p}\, f_0 X\, Y, \tag{2.35}$$

and $\tilde{a}(\mathbf{k},\mathbf{v}) \equiv e^{-t(nI-i\mathbf{k}\cdot\mathbf{v})}$. After very long and tedious calculations, the leading term of the density-density fluctuation for large $|r-r'|$ represents long range correlations

$$(\delta n(\mathbf{r})\delta n(\mathbf{r}'))_{ne} \sim (\delta n(\mathbf{r})\delta n(\mathbf{r}')\rangle_e - a\frac{3}{80}\frac{n}{\pi\Gamma}\frac{(x-x')(y-y')}{(r-r')^3}, \tag{2.36}$$

where Γ is a sound damping constant and n is the equilibrium density. The detailed calculations are discussed in Appendix A. From this result, we can see the algebraic decay of the density fluctuation in space. The exponent of

the spatial decay is equivalent to the result obtained from the phenomenological method of Lutsko and Dufty [18]. Recently, light scattering experiments were performed with temperature gradients [4,29] and the results confirm the existence of the long range correlations.

The result we calculated is only valid at the low density limit and near equilibrium. For states far from equilibrium, we should include the second and higher order terms from (2.20). This leads to increasingly complex expressions involving multi-time, multi-variable correlation functions. At present, it does not appear to be a practical approach. In the next chapter, we are going to construct the kinetic "model" equations related to the equations of transport and fluctuations to find a way to circumvent these difficulties, and so finally to be able to calculate the transport and fluctuations for states far from equilibrium.

CHAPTER 3
KINETIC MODELS FOR CORRELATIONS

Kinetic theory traditionally provides an equation for the single particle reduced distribution function (e.g. the Boltzmann equation at low density). However, kinetic theory can be extended to obtain equations for correlation functions as well by applying the same many-body methods used to derive an equation for the distribution function. In the first section, these equations for the distribution function and the pair correlation functions at low density are recalled. While these equations provide a complete description of nonequilibrium phenomena at low density, it is recognized that their application is very difficult except for limited cases such as states near equilibrium. To allow a practical study of states far from equilibrium, a well known kinetic model equation for the distribution function is adopted. In the second section, a self-consistent kinetic model for the correlation function also is obtained by exploiting the exact structural relationship between the kinetic equation for the distribution function and those for the correlation functions. In the third section, these model equations are used to describe fluctuations in nonequilibrium steady states. To illustrate the practical advantages of these equations, existing results for correlations at and near equilibrium are derived simply and directly in the last section.

3.1 Kinetic Equations for Correlations

Kinetic theory is one of the starting points to explain nonequilibrium transport properties and fluctuations. It describes the dynamics of the system in terms of reduced distribution functions. If the interaction potential between particles is short ranged, and the system is limited to low density, then the equation for the single particle distribution function is the Boltzmann equation. The same low density approximation method used to derive the Boltzmann equation can be extended to obtain kinetic equations for the equal and multi-time phase space correlation functions (see Appendix B). Equal and two time correlation functions are the most important quantities to study nonequilibrium fluctuations because these quantities are related to the physical observables and they can be measured in the laboratory. In this section, the equations for equal and two time correlation functions are reviewed within the low density approximation. [19, 30, 31]

Certain velocity moments of the distribution function are the hydrodynamic variables (density, temperature and velocity) and, similarly, the corresponding moments of the phase space correlation functions are the hydrodynamic fluctuations. Consequently the kinetic theory considered below can be used to obtain a hydrodynamic description as well. This is discussed in Chapters 4-6.

The system considered here is a low density gas of point particles interacting via a short ranged potential. Let $y = \{\mathbf{r}, \mathbf{v}\}$ denote the position and velocity of a point in the single phase space. A set of the microscopic densities is introduced as

$$\hat{f}(y,t) \equiv \sum_{i=1}^{N} \delta(y - x_i(t)), \tag{3.1}$$

$$\hat{f}(y,t;y',t') \equiv \hat{f}(y,t)\hat{f}(y',t'), \tag{3.2}$$

$$\hat{f}(y_1,y_2,t) \equiv \hat{f}(y_1,t;y_2,t) - \delta(y_1-y_2)\hat{f}(y_1,t), \tag{3.3}$$

where $x_i(t) \equiv \{\mathbf{q}_i(t), \mathbf{v}_i(t)\}$ denotes the position and velocity for particle i at time t. The single particle phase space density given in (3.1) can be generalized to a multi-point density according to

$$\hat{f}^{(s)}(y_1,\cdots,y_s,t) \equiv \sum_{i_1\neq i_2\neq\cdots} \cdots \sum_{\cdots\neq i_s} \prod_{\alpha=1}^{s} \delta(y_\alpha - x_{i\alpha}(t)). \tag{3.4}$$

The average of this microscopic density is the s-particle reduced distribution function,

$$f^{(s)}(y_1,\cdots y_s,t) \equiv (\hat{f}^{(s)}(y_1,\cdots,y_s,t)\rangle. \tag{3.5}$$

The angle brackets denote an ensemble average over some specified initial ensemble. For simplicity, we chose the initial time to be zero without loss of generality. Correlations at two phase points and times are defined by

$$\begin{aligned} C(y,t;y',t') &\equiv f(y,t;y',t') - f(y,t)f(y',t') \\ &= \langle\Big(\hat{f}(y,t) - (\hat{f}(y,t))\Big)\,\hat{f}(y',t')\rangle. \end{aligned} \tag{3.6}$$

Often a single time pair correlation, $G(y_1,y_2,t)$, is used for equal time correlations

instead of $C(y,t;y',t)$,

$$\begin{aligned} G(y_1,y_2,t) &\equiv f(y_1,y_2,t) - f(y_1,t)f(y_2,t) \\ &= C(y_1,t;y_2,t) - \delta(y_1-y_2)f(y_1,t). \end{aligned} \tag{3.7}$$

Since $G(y_1,y_2,t)$ is the correlation function without the $\delta(y_1-y_2)$ function, it represents the "true" correlation. We note that for observables of the form,

$$A(t) = \sum_{i=1}^{N} a_i, \quad B(t) = \sum_{i=1}^{N} b_i, \tag{3.8}$$

their averages and fluctuations are related to $f^{(1)}$ and $C(y,t;y',t')$ by Eqs.(1.1) and (1.2) according to

$$(A(t))_{t_0} = \int dy a(y,t) f^{(1)}(y,t), \tag{3.9}$$

$$(\delta A(t)\delta B(t'))_{t_0} = \int dy dy' a(y,t) b(y',t') C(y,t;y',t'). \tag{3.10}$$

The reduced distribution functions obey the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy. The equations of the hierarchy can be closed by using a systematic expansion in powers of a parameter that is small at low density. These low density approximations provide the equations for transport and correlation functions at equal and two time. The detailed derivation can be found in Appendix B. The kinetic equations are the following,

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla\right) f(y,t) = J(y|f(t)), \tag{3.11}$$

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla - \Lambda\right) C(y,t;y',t') = 0, \tag{3.12}$$

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_1\cdot\nabla_1 - \Lambda_1 + \mathbf{v}_2\cdot\nabla_2 - \Lambda_2\right) C(y_1,t;y_2,t) = B(y_1,y_2|f(t)), \tag{3.13}$$

where $J(y|f(t))$ is the nonlinear Boltzmann collision operator

$$J(y|f(t)) = \int dy' T(1,2) f(y,t) f(y',t). \tag{3.14}$$

And $T(1,2)$ is a binary scattering operator defined in (B.2). These three kinetic equations are a fundamental basis for the theoretical study of the transport and fluctuations in general nonequilibrium states at low density. In principle, these equations are solvable because they are linear equations.

The Eq.(3.11) is the well known Boltzmann equation, and it gives a familiar solution, the Maxwell Boltzmann distribution at equilibrium. Since this does not couple to the other equations, it is self-solvable if an initial condition and proper boundary condition are given. However, it is very difficult to solve practically except near equilibrium because of the nonlinear collision operator.

The kinetic equation for the two time correlation function in (3.12) applies for $t \geq t'$ and it represents a response at time t to a small perturbation from the state which is described with $f(y',t')$. An operator Λ in (3.12) has a functional

relationship with the Boltzmann collision operator such as

$$\Lambda h(y) = \int dy_1 \frac{\delta J(y|f(t))}{\delta f(y_1,t)} h(y_1). \tag{3.15}$$

From this relation, we can see that the equation of two time correlation functions has same structure as that for the distribution function linearized around $f(t)$ as the reference state. This also verifies a generalization of Onsager's assumption on the regression of fluctuations in the nonequilibrium state [32, 33]. In order to solve Eq.(3.12), an initial condition should be provided which is the equal time correlation function, $C(y_1,t;y_2,t)$. The equation for the equal time correlation function $C(y_1,t;y_2,t)$ is derived from (3.13). This equation consists of two of the same Λ operators and a new source term, $B(y_1,y_2,t)$, which is given by

$$B(y_1,y_2|f) = \gamma(y_1,y_2|f) + \delta(y_1-y_2)J(y_1|f) - (\Lambda_1+\Lambda_2)\delta(y_1-y_2)f(y_1,t), \tag{3.16}$$

where $\gamma(y_1,y_2,t)$ is defined by

$$\gamma(y_1,y_2|f) \equiv T(1,2)f(y_1,t)f(y_2,t), \tag{3.17}$$

and $T(1,2)$ defines the binary scattering operator for a two-particle collision (see Eq.(B.5)). For local equilibrium state, $f = f_\ell$, it is easily seen from the Eq.(B.5) that $\gamma(y_1,y_2|f_\ell)$ vanishes and so does $J(y|f_\ell)$. Then the remaining source term $B(y_1,y_2|f_\ell)$ simplifies to

$$B(y_1,y_2|f_\ell) = -(\Lambda_1+\Lambda_2)\delta(y_1-y_2)f_\ell(y_1,t). \tag{3.18}$$

This equation shows a Fluctuation (B) and Dissipation (Λ operator) relation in a local equilibrium state, in agreement with the one derived by Bixon and Zwanzig [34] and by Fox and Uhlenbeck [35]. However in a nonequilibrium state, $\gamma(y_1, y_2|f(t))$ and $\delta(y_1 - y_2)J(y_1|f(t))$ are no longer zero. These nonvanishing terms are responsible for different nonequilibrium correlation effects. Indeed $\gamma(y_1, y_2|f(t))$ is a true source term of unusual nonequilibrium fluctuations such as long range spatial correlations. This long range correlation effect will be studied further in section (3.4.2). The meaning of the true source term can be seen clearly if the kinetic equation for $G(y_1, y_2, t)$, defined in (3.7) is derived. The correlation $G(y_1, y_2|f)$ is a pair correlation function and can be called a true correlation function since it is zero at local equilibrium state. The kinetic equation for $G(y_1, y_2, t)$ is

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_1 \cdot \nabla_1 - \Lambda_1 + \mathbf{v}_2 \cdot \nabla_2 - \Lambda_2\right) G(y_1, y_2, t) = \gamma(y_1, y_2|f(t)). \qquad (3.19)$$

The inhomogeneous term $\gamma(y_1, y_2|f)$ plays the role of a source for the correlation functions $G(y_1, y_2, t)$. This source term defined in (3.17) represents velocity change through a single binary collision without spatial correlations. In a nonequilibrium state it represents a violation of a detailed balance and generates long range nonequilibrium fluctuations.

Since the kinetic equations for correlations are all functionals of the solution to the Boltzmann equation, once the solution to the Boltzmann equation is found, the correlations also can be determined in general. However the set of equations is still highly complicated. In next section, we will use a BGK kinetic model for

the Boltzmann collision operator, and this model will be used to construct the associated kinetic models for correlations. These three model kinetic equations admit more practical applications.

3.2 Kinetic Models for Correlations

Exact solutions to the Boltzmann equation are very limited because of the nonlinear collision operator term. Therefore kinetic models have been proposed for the Boltzmann collision operator by replacing it with a simpler, more tractable, operator. The most famous model of these is a single relaxation time model due to Bhatnager, Gross and Krook (BGK model) [23]. The essential qualities of this model are its preservation of the exact equilibrium solution and all five conservation laws. In this section, the BGK model for the Boltzmann equation is extended to a model for the dynamics of correlations.

When the kinetic models for kinetic equations are developed, several exact properties of the kinetic equations (3.11)-(3.13) should be preserved in addition to their structural relationships. A first essential property of $J(y|f)$ is its stationary point at the local equilibrium distribution f_ℓ,

$$J(y|f_\ell(t)) = 0, \tag{3.20}$$

where f_ℓ has the form

$$f_\ell(y,t) = exp\left(\sum_{\alpha=1}^{5} z_\alpha(\mathbf{r},t)\psi_\alpha(\mathbf{v})\right). \tag{3.21}$$

The five functions $z_\alpha(\mathbf{r}, t)$ are arbitrary at this point, and $\psi_\alpha(\mathbf{v})$ are the collisional invariants of the nonlinear Boltzmann operator,

$$\psi_\alpha(\mathbf{v}) = \{1, \mathbf{v}, v^2\}. \tag{3.22}$$

A second property of the collision operator follows from the conservation laws,

$$\int d\mathbf{v}\, \psi_\alpha(\mathbf{v}) J(y|f(t)) = 0. \tag{3.23}$$

These two properties of the Boltzmann collision operator also are relevant to the kinetic equations for correlations via the relationship (3.15),

$$\Lambda(y, t|f_\ell, f_\ell) = 0, \tag{3.24}$$

$$\int d\mathbf{v}\, \psi_\alpha(\mathbf{v}) \Lambda(y, t|f, h) = 0. \tag{3.25}$$

Finally, the orthogonality condition for the collisional invariants of the source term $B(y_1, y_2|f(t))$ is an important property to be preserved, and is related to the conservation laws,

$$\int d\mathbf{v}_1\, \psi_\alpha(\mathbf{v}_1) B(y_1, y_2|f(t)) = 0. \tag{3.26}$$

The above three properties should be preserved in constructing kinetic models.

For the Boltzmann collision operator, the BGK kinetic model preserves the primary properties of collision operator, stationarity (3.20) and the conservation

laws (3.23),

$$J^{\mathrm{BGK}}(y,|f(t)) \equiv -\nu\left(f(t)-f_\ell(t)\right), \tag{3.27}$$

where ν is a collision frequency which depends on the particle interaction law. The conservation laws are imposed by choosing the arbitrary functions $z_\alpha(\mathbf{r},t)$ in the local equilibrium distribution to satisfy

$$\int d\mathbf{v}\,\psi_\alpha(\mathbf{v})(f(y,t)-f_\ell(y,t))=0. \tag{3.28}$$

This provides five equations defining the z_α as functionals of f.

A corresponding model for the operator Λ is obtained directly from (3.15) to give

$$\begin{aligned}\Lambda^{\mathrm{BGK}}h(y) &\equiv \int dy_1\left(\frac{\delta}{\delta f(y_1,t)}J^{BGK}(y|f(t))\right)h(y_1)\\ &= -\nu\left(h(y)-\int dy_1\,h(y_1)\frac{\delta}{\delta f(y_1,t)}f_l(y,t)\right).\end{aligned} \tag{3.29}$$

The functional dependence of f_l on f occurs entirely through the z_α. Therefore,

$$\frac{\delta}{\delta f(y_1,t)}f_l(y,t)=f_l(y,t)\psi_\alpha(\mathbf{v})\frac{\delta}{\delta f(y_1,t)}z_\alpha(\mathbf{r},t). \tag{3.30}$$

A summation convention over repeated Greek labels is assumed. The functional derivative in (3.30) is evaluated by using the conservation law property (3.28) and it gives the BGK model for Λ operator

$$\Lambda^{\mathrm{BGK}}h(y)=-\nu\left(1-P\right)h(y), \tag{3.31}$$

where $P(t)$ is a projection operator defined over functions $X(y)$ by

$$PX(y) = f_l(y,t)\psi_\alpha(\mathbf{v})g^{-1}_{\alpha\beta}(\mathbf{r},t)\int d\mathbf{v}_1\,\psi_\beta(\mathbf{v}_1)X(\mathbf{r},\mathbf{v}_1). \tag{3.32}$$

The detailed derivation for Λ^{BGK} is in Appendix C.

Next, for the equal time correlation function, a model for the source term $B(y_1,y_2|f)$ is required in addition to Λ^{BGK}. The primary constraint for constructing B^{BGK} is the orthogonality condition in (3.26). Therefore we first make the orthogonality of B to the collisional invariants explicit by inserting two orthogonal projections in (3.16),

$$\begin{aligned} B(y_1,y_2|f) = (1-P_1)(1-P_2)[&\gamma(y_1,y_2|f) + \delta(y_1-y_2)J(y_1|f) \\ &-(\Lambda_1+\Lambda_2)\delta(y_1-y_2)f(y_1)]. \end{aligned} \tag{3.33}$$

This result is still exact. To define the corresponding BGK model for B, we replace J and Λ by J^{BGK} and Λ^{BGK} *and* neglect $(1-P_1)(1-P_2)\gamma(y_1,y_2|f)$ (it is a choice we make for simplicity), leading to the result

$$B^{\mathrm{BGK}}(y_1,y_2|f) = \nu(1-P_1)(1-P_2)\delta(y_1-y_2)(f(y_1)+f_l(y_1)), \tag{3.34}$$

where use has been made of the property $(1-P_1)(1-P_2)(P_1+P_2)=0$. While the orthogonality condition is not sufficient to determine B^{BGK} uniquely, the choice (3.34) is consistent with the known form near equilibrium (3.18). With this B^{BGK} model, the kinetic model for the source term γ^{BGK} in the equation for G (3.19)

can be defined. The definition for B (3.16) is used

$$\gamma^{\mathrm{BGK}}(y_1, y_2|f) = B^{\mathrm{BGK}}(y_1, y_2|f) - \delta(y_1 - y_2)J^{\mathrm{BGK}}(y_1|f) \\ +(\Lambda_1^{\mathrm{BGK}} + \Lambda_2^{\mathrm{BGK}})\delta(y_1 - y_2)f(y_1). \tag{3.35}$$

Then the model for γ^{BGK} is

$$\gamma^{\mathrm{BGK}}(y_1, y_2|f) = \nu P_1 P_2 \delta(y_1 - y_2)[f(y_1) - f_\ell(y_1)], \tag{3.36}$$

where use has been made of the property $P_1(1 - P_2)f_\ell(y_2)\delta(y_1 - y_2) = 0$.

Now the extended BGK model for kinetic equations has been completed. Eqs.(3.11)-(3.13) are now replaced by

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla\right) f(y,t) = -\nu\left(f(y,t) - f_l(y,t)\right), \tag{3.37}$$

$$\left(\frac{\partial}{\partial t} + \mathcal{L}(t)\right) C(y,t;y',t') = 0, \tag{3.38}$$

$$\left(\frac{\partial}{\partial t} + \mathcal{L}_1(t) + \mathcal{L}_2(t)\right) C(y_1,t;y_2,t) = \nu(1-P_1)(1-P_2)\delta(y_1-y_2)(f(y_1,t)+f_l(y_1,t)), \tag{3.39}$$

where the operator $\mathcal{L}$ is defined by

$$\mathcal{L}(t) \equiv \mathbf{v}\cdot\nabla + \nu(1-P). \tag{3.40}$$

The equation for $G(y_1, y_2, t)$ also is written

$$\left(\frac{\partial}{\partial t} + \mathcal{L}_1(t) + \mathcal{L}_2(t)\right) G(y_1, t; y_2, t) = \gamma^{\mathrm{BGK}}(y_1, y_2 | f(t)). \tag{3.41}$$

Equations (3.37)-(3.39), or (3.41) provide the transport properties and fluctuations in nonequilibrium gas. Since these equations are derived without any restriction to near equilibrium states, these equations can be used for practical applications of transport and fluctuations far from equilibrium.

The equations can be solved by first solving the BGK-Boltzmann equation for given initial and boundary conditions. Once the solution to the transport equation is found, it is used to determine the operator $\mathcal{L}$ and the source term B or γ. To solve the two time correlation function equation for $t \geq t'$, for the initial value is needed at $t = t'$. This initial value is calculated from the solution to (3.39) or (3.41). In the next section, the formal solutions to the equations for the correlations are constructed with the assumption that the solution to the BGK-Boltzmann equation is known. The solution to the BGK-Boltzmann equation will be calculated in Chapter 4 for uniform shear flow as a special nonequilibrium state.

3.3 Steady State Correlations

The kinetic models developed above allow the study of correlations, once the solution to the Boltzmann equation is obtained. BGK-Boltzmann equation is still a highly nonlinear integro-differential equation due to the dependence of

f_ℓ on f. However, exact solutions of a Boltzmann equation for nonequilibrium steady states corresponding to heat and momentum transport have been obtained recently for planar geometries [36]. Since the system considered in this thesis is uniform shear flow, the exact solution to BGK-Boltzmann equation will be studied specifically in the next chapter. In this section, to illustrate the formal solutions to the correlation function equations (3.38, 3.39), we assume that a steady state distribution, f_s, is known. Then the formal solution to Eq.(3.38) is

$$C_s(y,t;y',0) = \int dy_1\, K(y,y_1,t) C_s(y_1,0;y',0), \tag{3.42}$$

$$K(y,y',t) \equiv \exp\{-\mathcal{L}t\}\,\delta(y-y'). \tag{3.43}$$

Stationarity has been used to choose $t' = 0$. The initial condition in (3.42) is determined from the stationary solution to the equal time correlation function equation, (3.39),

$$\begin{aligned} C_s(y,y') &= C_s(y,0;y',0) \\ &= \int_0^\infty d\tau \int dy_1 dy_2\, K(y,y_1,\tau) K(y',y_2,\tau) B^{\mathrm{BGK}}(y_1,y_2|f_s). \end{aligned} \tag{3.44}$$

The two formal solutions to the correlation equations are expressed in terms of the Green's function $K(y,y',t)$, defined in (3.43). The equation for this Green's function is

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla + \nu\right) K(y,y',t) = \nu f_s(y)\psi_\alpha(\mathbf{v}) K_\alpha(\mathbf{r},y',t), \tag{3.45}$$

with the initial condition $K(y, y', 0) = \delta(y - y')$. The functions $K_\alpha(\mathbf{r}, y', t)$ are defined by

$$K_\alpha(\mathbf{r}, y', t) \equiv g_{\alpha\beta}^{-1}(\mathbf{r}|f_s) \int d\mathbf{v}_1 \, \psi_\beta(\mathbf{v}_1) K(\mathbf{r}, \mathbf{v}_1, y', t). \tag{3.46}$$

The solution to (3.45) can be reduced to the corresponding ideal gas problem as follows. Integration of (3.45) gives

$$\begin{aligned} K(y, y', t) = {} & K_0(y, y', t) \\ & + \nu \int_0^t d\tau \int dy_1 \, K_0(y, y_1, t - \tau) f_s(y_1) \psi_\alpha(\mathbf{v}_1) K_\alpha(\mathbf{r}_1, y', \tau), \end{aligned} \tag{3.47}$$

where we have introduced

$$K_0(y, y', t) \equiv \exp\left[-(\mathbf{v} \cdot \nabla + \nu)\, t\right] \delta(y - y'). \tag{3.48}$$

The remaining set of five functions $K_\alpha(\mathbf{r}, y', t)$ is determined by substituting (3.47) into the right side of (3.46) to give

$$K_\alpha(\mathbf{r}, y', t) = K_{0\alpha}(\mathbf{r}, y', t) + \int_0^t d\tau \int d\mathbf{r}_1 I_{\alpha\beta}(\mathbf{r}, \mathbf{r}_1, t - \tau) K_\beta(\mathbf{r}_1, y', \tau), \tag{3.49}$$

with

$$K_{0\alpha}(\mathbf{r}, y', t) \equiv g_{\alpha\beta}^{-1}(\mathbf{r}|f_s) \int d\mathbf{v} \, \psi_\beta(\mathbf{v}) K_0(y, y', t), \tag{3.50}$$

and

$$I_{\alpha\beta}(\mathbf{r},\mathbf{r}_1,t) \equiv \nu\, g^{-1}_{\alpha\gamma}(\mathbf{r}|f_s) \int d\mathbf{v}d\mathbf{v}_1\, \psi_\gamma(\mathbf{v}) K_o(y,y_1,t) f_s(y_1)\psi_\beta(\mathbf{v}_1). \tag{3.51}$$

The quantity K_0 is determined entirely from the dynamics of the free streaming gas . Then $K_{0\alpha}$ and $I_{\alpha\beta}$ are obtained from integration, and the Green's function K is also calculated in (3.47). Finally, the equal time correlation function (3.42) and dynamic correlation function (3.44) can be calculated. Examples of this analysis are shown in the following sections for equilibrium states and stationary states near equilibrium. From the confirming results of these examples, the validity of kinetic models for B^{BGK} and γ^{BGK} is supported.

3.4 Examples

Two simple states are considered to illustrate the analysis of kinetic models in previous section. First the equilibrium state is considered, and from the same systematic analysis we calculate the extended hydrodynamic modes. The second example concerns a stationary state near equilibrium. The perturbation method about hydrodynamic field gradients is used to get a stationary state, and the equal time correlation function is calculated. In particular, the results of Chapter 2 for long range spatial correlations are recovered.

3.4.1 Equilibrium States

At equilibrium the distribution function is the local equilibrium state distribution. It is actually the Maxwell-Boltzmann distribution function,

$$f_e(v) = n\left(\frac{m}{2\pi k_B T}\right)^{3/2} \exp(-mv^2/2k_B T), \tag{3.52}$$

where n is the density m is the mass of the particle, k_B is the Boltzmann constant, and T is the temperature. The source term B^{BGK} given by (3.34) simplifies to

$$B^{\mathrm{BGK}}(y_1, y_2|f_e) = -(\mathcal{L}_1 + \mathcal{L}_2)\delta(y_1 - y_2)f_e(y_1), \tag{3.53}$$

in agreement with (3.18). Direct calculation from (3.43) and (3.44) gives the expected results for the low density equilibrium correlations,

$$C_e(y; y') = \delta(y - y')f_e(y). \tag{3.54}$$

Use of this as an initial value to (3.42) gives the two time correlation functions as

$$C_e(y, t; y', 0) = K(y, y', t)f_e(y'). \tag{3.55}$$

The Green's function is determined from (3.45)-(3.49). Fourier - Laplace transformation is used, giving

$$\begin{aligned}\tilde{C}_e(\mathbf{k}, \mathbf{k}', z; \mathbf{v}, \mathbf{v}') &\equiv \int d\mathbf{r}\, d\mathbf{r}'\, e^{i(\mathbf{k}\cdot\mathbf{r}+\mathbf{k}'\cdot\mathbf{r}')} \int_0^\infty dt\, \mathrm{e}^{-zt} C_e(y, t; y', 0) \\ &\equiv (2\pi)^3 \delta(\mathbf{k} + \mathbf{k}')\tilde{C}_e(\mathbf{k}, z|\mathbf{v}, \mathbf{v}').\end{aligned} \tag{3.56}$$

The correlation function is now written as

$$\tilde{C}_e(\mathbf{k}, z|\mathbf{v}, \mathbf{v}') = \tilde{K}(\mathbf{k}, z|\mathbf{v}, \mathbf{v}')f_e(\mathbf{v}'), \tag{3.57}$$

and the Green's function $\tilde{K}(\mathbf{k}, z|\mathbf{v}, \mathbf{v}')$ is

$$\begin{aligned}\tilde{K}(\mathbf{k}, z|\mathbf{v}, \mathbf{v}') = & R(\mathbf{k}, z|\mathbf{v})\delta(\mathbf{v} - \mathbf{v}') \\ & + \frac{\nu}{n}R(\mathbf{k}, z|\mathbf{v})R(\mathbf{k}, z|\mathbf{v}')f_e(v)\phi_\alpha(\mathbf{v})\phi_\beta(\mathbf{v}')B^{-1}_{\alpha\beta}(k, z),\end{aligned} \tag{3.58}$$

where

$$R(\mathbf{k}, z|\mathbf{v}) \equiv (z + \nu - i\mathbf{k}\cdot\mathbf{v})^{-1}, \tag{3.59}$$

$$B_{\alpha\beta}(k, z) \equiv \delta_{\alpha\beta} - \tilde{I}_{\alpha\beta}(k, z). \tag{3.60}$$

The functions ϕ_α are linear combinations of the summational invariants, ψ_α and are defined in Appendix D. The first term of the Green's function (3.58) describes the free streaming motion with a pure exponential damping by ν. The second term shows the dynamics of correlations determined by the singularity of the matrix $B^{-1}_{\alpha\beta}(k, z)$. The detailed form of matrix B is shown in Appendix D. The determinant of the matrix B gives five simple poles at $z_\alpha(k)$ which originated at $z(k = 0) = 0$. A pole at the origin represents a conserved quantity, so the five simple poles at finite k characterize five hydrodynamic modes which are two sound modes, a heat mode and two shear modes. Since there is no restriction on k, it is possible to calculate these poles not only at small k (Navier-Stokes order) but also at larger k. This defines the extended hydrodynamic modes. The

poles are calculated numerically for finite k, and it is found that for small k the dynamics of correlations is equivalent to that from the linearized Navier-Stokes equations. For large k, these extended modes exist up to some maximum values of k corresponding to wavelengths as compared to the mean free path. The real and

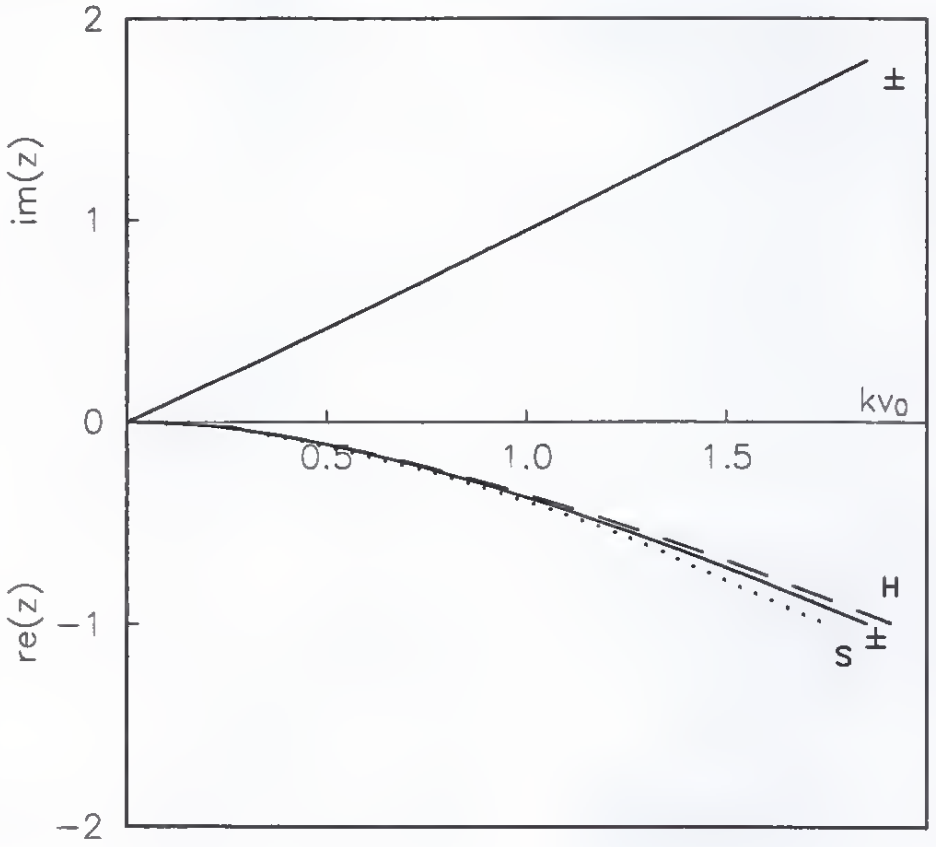

Figure 3.1: Real and imaginary parts of the extended hydrodynamic modes from the BGK model (in units of ν). $\pm$ indicates sound modes, H the heat mode and S the shear modes.

imaginary parts for the two propagating sound modes ($\pm$), , the heat diffusion mode (H), and the shear diffusion modes (s) are shown in Fig.3.1. In addition to the hydrodynamic modes, there are poles and branch points which approach $-\nu$ as $k \to 0$. These represent the kinetic modes with lifetimes of the order of ν^{-1} for all k.

This equilibrium dynamic correlations are well-studied field from the linearized Boltzmann equation using more complex models [37]. The analysis with our kinetic models for correlations shows that all qualitative features of fluctuations in equilibrium states are preserved.

3.4.2 Stationary States Near Equilibrium

As a second example, a stationary state near local equilibrium is considered. First, in order to solve the BGK-Boltzmann equation, the Chapman-Enskog approximation, which is a power series expansion in the gradients of the hydrodynamic variables, is used. The stationary solution, obtained by assuming small temperature and flow field gradients, is given by

$$f_s(y) \to f_l(y)\left[1 - \frac{1}{k_B T \nu}(T^{-1}\frac{\partial T}{\partial r_i}S_i(\mathbf{v}) + \frac{\partial u_i}{\partial r_j}D_{ij}(\mathbf{v}))\right]. \tag{3.61}$$

Here $T(\mathbf{r})$ is the temperature, $\mathbf{u}(\mathbf{r})$ is the flow field, and

$$\mathbf{S}(\mathbf{v}) \equiv \mathbf{V}(\frac{1}{2}mV^2 - \frac{5}{2}k_B T), \tag{3.62}$$

$$D_{ij}(\mathbf{v}) \equiv m(V_i V_j - \frac{1}{3}V^2\delta_{ij}), \tag{3.63}$$

where $\mathbf{V}(\mathbf{r}) \equiv \mathbf{v} - \mathbf{u}(\mathbf{r})$ is the peculiar velocity.

The equal time correlation function is calculated in terms of an integral representation for the solution to (3.41) rather than (3.39) in order to see the difference from equilibrium correlations more directly. It is

$$G_s(y_1, y_2) = \int_0^\infty dt\, e^{-(\mathcal{L}_1+\mathcal{L}_2)t}\gamma(y_1, y_2|f_s). \tag{3.64}$$

This shows a signature of long ranged spatial correlations which arise from the hydrodynamic spectrum of $\mathcal{L}$. It can be calculated further by using the hydrodynamic eigenfunctions of $\mathcal{L}$ to the lowest order in the gradients. The eigenfunctions are proportional to the summational invariants, ψ_α, so

$$\begin{aligned} G_s \longrightarrow & \int_0^\infty dt\, \mathrm{e}^{-(\mathcal{L}_1+\mathcal{L}_2)t}\delta(\mathbf{r}_1 - \mathbf{r}_2)M_{\alpha\beta}\psi_\alpha(\mathbf{v}_1)\psi_\beta(\mathbf{v}_2)f_l(y_1)f_l(y_2) \\ & = (\mathcal{L}_1 + \mathcal{L}_2)^{-1}\delta(\mathbf{r}_1 - \mathbf{r}_2)M_{\alpha\beta}\psi_\alpha(\mathbf{v}_1)\psi_\beta(\mathbf{v}_2)f_l(y_1)f_l(y_2), \end{aligned} \tag{3.65}$$

where

$$M_{\alpha\beta}\delta(\mathbf{r}_1 - \mathbf{r}_2) \equiv g^{-1}_{\alpha\sigma}g^{-1}_{\beta\nu}\int d\mathbf{v}_1 d\mathbf{v}_2 \psi_\sigma(\mathbf{v}_1)\psi_\nu(\mathbf{v}_2)\gamma(y_1, y_2|f). \tag{3.66}$$

In Fourier representation, the eigenvalues of $\mathcal{L}$ lead to terms $\propto (\lambda_\alpha(k) + \lambda_\beta(k))^{-1}$ which lead to slow algebraic decay in configuration space. This is a very interesting phenomena because there are no long ranged correlations in the equilibrium state. These long ranged correlations near equilibrium have been verified

perturbatively [2] and recently accurate experimental results [4, 29, 38] are supporting the existence of the long ranged correlations. The coefficients $M_{\alpha\beta}$ can be calculated easily and explicitly . First, $\gamma(y_1, y_2|f)$ is found from (3.36),

$$\gamma^{BGK}(y_1, y_2|f_s) = -P_1P_2\delta(y_1 - y_2)f_l(v_1)\left[\frac{1}{k_BT}(T^{-1}\frac{\partial T}{\partial r_i}S_i(\mathbf{v_1}) + \frac{\partial u_i}{\partial r_j}D_{ij}(\mathbf{v}_1))\right]. \tag{3.67}$$

Next, the result for $M_{\alpha\beta}$ is calculated to be

$$M_{\alpha\beta} = -\left[\frac{1}{k_BT}(T^{-1}\frac{\partial T}{\partial r_i}S_{\alpha\beta,i} + \frac{\partial u_i}{\partial r_j}D_{\alpha\beta,ij})\right], \tag{3.68}$$

where

$$S_{\alpha\beta,i} \equiv g^{-1}_{\alpha\sigma}g^{-1}_{\beta\nu}\int d\mathbf{v} f_l(v)\psi_\sigma(\mathbf{v})\psi_\nu(\mathbf{v})S_i(\mathbf{v}), \tag{3.69}$$

$$D_{\alpha\beta,ij} \equiv g^{-1}_{\alpha\sigma}g^{-1}_{\beta\nu}\int d\mathbf{v} f_l(v)\psi_\sigma(\mathbf{v})\psi_\nu(\mathbf{v})D_{ij}(\mathbf{v})). \tag{3.70}$$

These results are exactly the same as those obtained from the true kinetic theory (3.19) [39].

With this general result, the density correlation function can be calculated for uniform shear flow in order to compare the result with the one we got from the Liouville equation in Chapter 2. The density correlation function is defined by

$$\begin{aligned}
&\langle\delta n(\mathbf{r}_1)\delta n(\mathbf{r}_2)\rangle \\
&= \int d\mathbf{v}_1 d\mathbf{v}_2\, C_s(y_1, y_2) &(3.71)\\
&= n\delta(\mathbf{r}_1 - \mathbf{r}_2) + \int_0^\infty dt \int d\mathbf{v}_1 d\mathbf{v}_2 e^{-(\mathcal{L}_1+\mathcal{L}_2)t}\gamma(y_1, y_2|f_s). &(3.72)
\end{aligned}$$

The first term of Eq.(3.72) represents equilibrium density fluctuations and is same as (2.26) with very short range correlation. The second term of Eq.(3.72) represents the second term of Eq.(2.25) at low density. By using the coefficients $M_{\alpha\beta}$ as defined in (3.68), the second term is rewritten as

$$\begin{aligned}
&\int_0^\infty dt \int d\mathbf{v}_1 d\mathbf{v}_2\, e^{-(\mathcal{L}_1+\mathcal{L}_2)t}\gamma(y_1,y_2|f_s) \\
&= \delta(\mathbf{r}_1-\mathbf{r}_2)M_{\alpha\beta}\int_0^\infty dt \int d\mathbf{v}_1\, e^{-\mathcal{L}_1 t}\psi(\mathbf{v}_1)f_\ell(y_1) \\
&\quad \times \int d\mathbf{v}_2\, e^{-\mathcal{L}_2 t}\psi(\mathbf{v}_2)f_\ell(y_2). \qquad (3.73)
\end{aligned}$$

The coefficients $M_{\alpha\beta}$ in (3.68) have only one velocity gradient term in uniform shear flow,

$$M_{\alpha\beta} = -\frac{a}{k_B T} D_{\alpha\beta,xy}. \qquad (3.74)$$

A Fourier transformation is performed for the density correlations. The operator $\mathcal{L}$ becomes the $\tilde{\mathcal{L}} = -i\mathbf{k}\cdot\mathbf{v} + \nu(1-P)$. The hydrodynamic eigenvalues and eigenvectors of the operator $\tilde{\mathcal{L}}$ are equal to the hydrodynamic spectrum of the inhomogeneous linearized Boltzmann operator which can be found in (A.5)-(A.9). Also for simplicity, the collisional invariants ψ_α are chosen to be the same orthonormal set $\{\phi_\alpha\}$ as was used in equilibrium analysis in the first example, Eq. (D.2). By using the lowest order eigenvectors of $\tilde{\mathcal{L}}$ and the nonzero elements of $M_{\alpha\beta}$, the density correlation function is found to be

$$\begin{aligned}
&\langle \delta n(\mathbf{r}_1)\delta n(\mathbf{r}_2)\rangle \\
&= n\delta(\mathbf{r}_1-\mathbf{r}_2) - \frac{1}{2\pi^3}2n\,a\int d\mathbf{k} e^{-i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)}\frac{k_x k_y}{k^2}\left[\frac{3}{20\Gamma k^2}+\frac{3}{10}\frac{\Gamma k^2}{\Gamma^2 k^4+k^2c^2}\right]
\end{aligned}$$

(3.75)

$$= n\,\delta(\mathbf{r}_1 - \mathbf{r}_2) - \frac{3}{80}\frac{a\,n}{\pi\Gamma}\frac{(x_1 - x_2)(y_1 - y_2)}{(r_1 - r_2)^3} + \text{higher order.} \tag{3.76}$$

This result is exactly same as the one in (2.36) which was obtained in Chapter 2. This proves that the BGK-kinetic models preserve a correct description of fluctuation phenomena in stationary state and near equilibrium, and they also provide a simpler and more practical approach to the problem.

CHAPTER 4
TRANSPORT EQUATIONS FOR UNIFORM SHEAR FLOW

Kinetic model equations for transport and fluctuations were developed in the last chapter. We now specialize those equations to uniform shear flow. In this chapter, the BGK-Boltzmann equation for the distribution function, f, is examined to study transport properties of the system. The stationary reference state solution will be determined and discussed. Later, a "normal" solution for states near this stationary state is obtained using a modified Chapman-Enskog method. This normal solution then is used to calculate the average heat and momentum fluxes, which obtains a hydrodynamic description. These hydrodynamic equations are accurate to second order in spatial gradients relative to uniform shear flow state, but there is no restriction on value of the shear rate. The shear rate dependent generalized transport coefficients are given explicitly.

4.1 Stationary State Solution

In the last chapter, a more practical and theoretical description of nonequilibrium phenomena has been given by the BGK model equations (3.37)-(3.41). However the first of these equations, the BGK-Boltzmann equation, is highly nonlinear and difficult to solve in general. One of the few cases for which an exact solution is known is that for uniform shear flow. Consequently, in the remainder of this thesis, attention will be restricted to uniform shear flow and states near

uniform shear flow. The uniform shear state is a planar flow whose x-component of the flow velocity has a gradient along the y-axis, $u_i = a_{ij} r_j$, $a_{ij} = a\,\delta_{ix}\delta_{jy}$, where a is a constant shear rate. In addition, the density n and temperature T are spatially uniform. This state is generated by a periodic boundary condition in the local Lagrangian frame [6], so there is no boundary layer, as there is for planar Couette flow [40]. Due to the simplicity of uniform shear flow state at the macroscopic level, it has been studied extensively as a prototype of nonequilibrium states far from equilibrium in theory [25, 41, 42] and in computer simulations [7–9, 26]. The boundary driven shear leads to viscous heating. For practical purposes, it is useful to introduce a uniform "thermostat" to control this heating and establish a steady state. This is done in most simulation studies.

Consider first the BGK-Boltzmann equation for a general nonequilibrium state,

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla_r + \nabla_v m^{-1}\cdot\mathbf{F}_{ext}\right) f = -\nu(f - f_\ell), \tag{4.1}$$

where $\mathbf{F}_{ext}$ which serves as a thermostat, is an external force applied on each particle. There are several thermostats that have been used in both theory and computer simulations. We choose here a force proportional to the velocity relative to the actual flow field and it is in the form of

$$\mathbf{F}_{ext}(\mathbf{v}, t) = -m\lambda(\mathbf{v} - \mathbf{u}(\mathbf{r}, t)). \tag{4.2}$$

The proportional "constant" λ is determined by requiring stationarity of the system, and may depend on the density, temperature and shear rate. The parameter

ν in the (4.1) is a collision frequency which depends on an interaction law. This frequency is a function of the density and temperature. At low density, it can be written as

$$\nu \sim nT^b, \tag{4.3}$$

when the potential has a form of $V(r) \sim r^{-l}$, with $b = 1/2 - 2/l$. In the case of Maxwell molecules ($l = 4$), b is zero so ν becomes independent of temperature. For the hard sphere case, l tends to infinity resulting in a value for b of $1/2$. Also, f_ℓ in (4.1) is the local equilibrium distribution function of (3.21), written more explicitly as

$$f_\ell(\mathbf{r}, \mathbf{v}, t) = n(\mathbf{r}, t) \left(\frac{m}{2\pi k_B T(\mathbf{r}, t)} \right)^{3/2} \exp\left(-\frac{m}{2k_B T(\mathbf{r}, t)} [\mathbf{v} - \mathbf{u}(\mathbf{r}, t)]^2 \right). \tag{4.4}$$

The hydrodynamic fields are defined by

$$n(\mathbf{r}, t) = \int d\mathbf{v}\, f(\mathbf{r}, \mathbf{v}, t), \tag{4.5}$$

$$n(\mathbf{r}, t)\mathbf{u}(\mathbf{r}, t) = \int d\mathbf{v}\, \mathbf{v} f(\mathbf{r}, \mathbf{v}, t), \tag{4.6}$$

$$\frac{3}{2} n(\mathbf{r}, t) k_B T(\mathbf{r}, t) = \int d\mathbf{v}\, \frac{1}{2} m(\mathbf{v} - \mathbf{u}(\mathbf{r}, t))^2 f(\mathbf{r}, \mathbf{v}, t), \tag{4.7}$$

which identifies n as the density, T as the temperature and $\mathbf{u}$ as the flow velocity.

The scales of interest are for the distances larger than the mean free path and for times longer than the mean free time. In this regime, the system is characterized by conserved hydrodynamic variables (such as density, momentum and energy). The local conservation laws are obtained from the Boltzmann equation

by integration over the velocities with summational invariants $(1, \mathbf{v}, v^2)$ to get

$$\frac{\partial n}{\partial t} + \nabla \cdot n\mathbf{u} = 0, \tag{4.8}$$

$$\frac{3}{2} n k_B \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) T + \nabla \cdot \mathbf{q} + t_{ij} \frac{\partial u_j}{\partial r_i} = w, \tag{4.9}$$

$$\frac{\partial u_i}{\partial t} + \mathbf{u} \cdot \nabla u_i + \frac{1}{\rho} \frac{\partial t_{ij}}{\partial r_j} = 0, \tag{4.10}$$

where n, T and $\mathbf{u}$ are the density, temperature and flow velocity. Also, t_{ij} is the pressure tensor,

$$t_{ij} = \int d\mathbf{v}\, m(v_i - u_i)(v_j - u_j) f, \tag{4.11}$$

and $\mathbf{q}$ is the heat flux,

$$\mathbf{q} = \int d\mathbf{v} \frac{1}{2} m(v - u)^2 (\mathbf{v} - \mathbf{u}) f. \tag{4.12}$$

The inhomogeneous term w in the temperature equation is due to the external nonconservative force representing the thermostat, and is written as

$$w = -3\lambda n k_B T. \tag{4.13}$$

The external force does not appear in the velocity equation since the average of (4.2) vanishes.

Now uniform shear flow is considered. It is useful to express the kinetic equation (4.1) in terms of the velocity in the local rest frame, defined by $v_i' = v_i - a_{ij} r_j$. In this frame, the macroscopic uniform shear state becomes spatially

homogeneous. Consequently, we look for a stationary solution to Eq.(4.1) of the form

$$f(\mathbf{r}, \mathbf{v}, t) = f_s(\mathbf{v}'). \tag{4.14}$$

The equation for f_s becomes,

$$\left(-a_{ij}v'_j\frac{\partial}{\partial v'_i} - \nabla_{v'}\cdot m^{-1}\mathbf{F}_{s,ext}(\mathbf{v}')\right) f_s(\mathbf{v}') = -\nu_s(f_s - f_{s\ell}), \tag{4.15}$$

where s denotes stationary and $f_{s\ell}$ is a stationary local equilibrium distribution function (Maxwell-Boltzmann distribution) with the hydrodynamic fields for uniform shear flow. The solution to Eq.(4.15) is

$$f_s(\mathbf{v}') = \nu\int_0^\infty d\tau\, e^{-\nu\tau}\mathrm{e}^{\tau L}f_\ell(\mathbf{v}'). \tag{4.16}$$

where L is the velocity operator,

$$L = a_{ij}v'_j\frac{\partial}{\partial v'_i} + \lambda\frac{\partial}{\partial v'_i}v'_i. \tag{4.17}$$

For an arbitrary function of $\mathbf{v}$, $X(\mathbf{v})$, it has the property,

$$e^{tL}X(\mathbf{v}) = \mathrm{e}^{3\lambda t}X(\mathrm{e}^{t\lambda}\Lambda_{ij}(-t)v_j), \tag{4.18}$$

where $\Lambda_{ij}(t) = \delta_{ij} - a_{ij}t$. Therefore the stationary solution can be written

$$f_s(\mathbf{v}') = \nu\int_0^\infty dt\,\mathrm{e}^{-t(\nu-3\lambda)}f_{s\ell}(\mathrm{e}^{\lambda t}\Lambda_{ij}(-t)v'_j). \tag{4.19}$$

The parameter λ is determined from the temperature equation (4.9) by requiring $\frac{\partial T}{\partial t} = 0$ and it is found that

$$\lambda = \frac{a\, t_{s,xy}}{3nk_B T_s}. \tag{4.20}$$

The components of the momentum flux can be calculated from Eq.(4.11) by direct integration to get

$$t_{s,xx} = p_s + \frac{4\lambda}{2\lambda + \nu} p_s, \tag{4.21a}$$

$$t_{s,xy} = -\frac{\nu a}{(2\lambda + \nu)^2} p_s, \tag{4.21b}$$

$$t_{s,yy} = p_s - \frac{2\lambda}{2\lambda + \nu} p_s, \tag{4.21c}$$

$$t_{s,zz} = t_{s,yy}, \tag{4.21d}$$

where $p_s = n_s k_B T_s$, $t_{s,ij} = t_{s,ji}$ and all other elements of $t_{s,ij}$ are zero. Use of $t_{s,xy}$ in (4.20) gives the equation to fix $\lambda(a)$,

$$3\lambda(2\lambda + \nu)^2 = \nu a^2. \tag{4.22}$$

This equation has one real solution and two complex conjugate solutions. The physically relevant real value is

$$\lambda = \frac{2}{3} \sinh[\cosh^{-1}(1 + 9\frac{a^2}{\nu^2})/6]^2. \tag{4.23}$$

From these expressions for the momentum fluxes, the shear viscosity $\eta(a)$ and

viscometric functions $\Psi_1(a)$, $\Psi_2(a)$ are determined to be

$$\eta(a) \equiv -\frac{t_{xy}}{a} = \frac{\nu}{(2\lambda+\nu)^2} p_s, \tag{4.24}$$

$$\Psi_1(a) \equiv \frac{t_{yy}-t_{xx}}{a^2} = -\frac{6\lambda}{a^2(2\lambda+\nu)} p_s, \tag{4.25}$$

$$\Psi_2(a) \equiv \frac{t_{zz}-t_{yy}}{a^2} = 0, \tag{4.26}$$

where all of the shear rate dependence occurs through $\lambda = \lambda(a)$ in (4.23). The same integration can be done for heat flux in (4.12), and it is found to vanish, as expected. Therefore (4.24)-(4.26) describe all the transport properties for the reference state of the uniform shear flow. The Figure 4.1 shows $\eta^*(a^*) \equiv \nu\eta/p_s$ and $\Psi_1^*(a^*) \equiv \nu^2\Psi_1/p_s$ as a function of $a^* \equiv a/\nu$. The results agree with previous studies [43, 44]. They exhibit strong rheological effects at large shear rates, even though we consider a simple gas. The transport coefficients behave for small shear rate as

$$\eta = \left(1 - \frac{4\,a^2}{3\,\nu^2} + \frac{28\,a^4}{9\,\nu^4} + \cdots\right)\frac{p_s}{\nu}, \tag{4.27}$$

$$\Psi_1 = \left(-2 + 4\frac{a^2}{\nu^2} - \frac{32\,a^4}{3\,\nu^4} + \cdots\right)\frac{p_s}{\nu^2}, \tag{4.28}$$

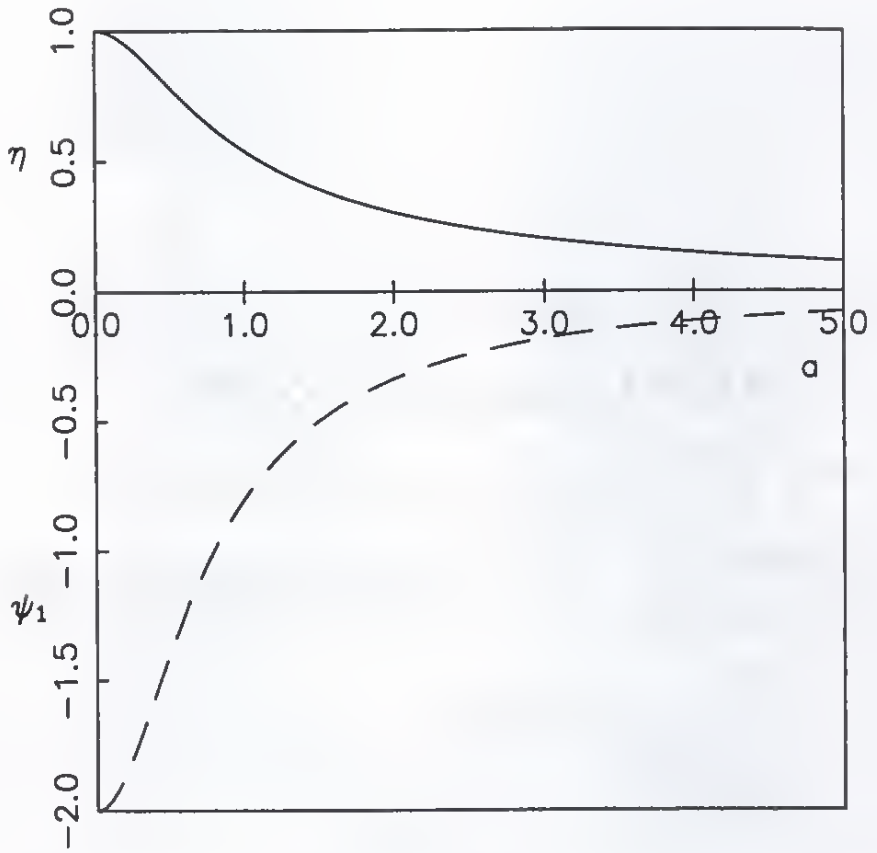

Figure 4.1: Shear viscosity $\eta(a)$(solid line) and viscometric function $\Psi(a)$ (dashed curve) are shown as function of a. η is in unit of p_s/ν, Ψ is in unit of p_s/ν^2 and a is in unit of ν.

and for large a as

$$\eta = \left(\frac{a}{\nu}\right)^{-4/3}\left(\left(\frac{3}{2}\right)^{2/3} - \left(\frac{a}{\nu}\right)^{-2/3} + \frac{1}{9}\left(\frac{3}{2}\right)^{4/3}\left(\frac{a}{\nu}\right)^{-4/3} + \cdots\right)\frac{p_s}{\nu}, \quad (4.29)$$

$$\Psi_1 = -\left(\frac{a}{\nu}\right)^{-2}\left(3 - 3\left(\frac{3}{2}\right)^{1/3}\left(\frac{a}{\nu}\right)^{-2/3} + \left(\frac{3}{2}\right)^{2/3}\left(\frac{a}{\nu}\right)^{-4/3} + \cdots\right)\frac{p_s}{\nu^2}. \quad (4.30)$$

Now all hydrodynamic variables and fluxes are known for the stationary uniform shear state. Our next interests are to study fluctuations in this state, and to see the behavior of states which deviate from the stationary state by small spatial gradients. In the next section, a variant of the Chapman-Enskog expansion method is introduced to the BGK-Boltzmann equation to find a "normal" solution for these latter states.

4.2 Normal Solution

Our objective here is to find a solution which describes small perturbations relative to stationary uniform shear flow due to spatial gradients in the hydrodynamics fields. Since the stationary state is homogeneous in the local rest frame, it is convenient to continue using the relative velocity $\mathbf{v}' = \mathbf{v} - \mathbf{u}_s$. The BGK-Boltzmann equation is then written as

$$\left(\frac{\partial}{\partial t} + (v_i' + a_{ij}r_j)\frac{\partial}{\partial r_i} - L(v',a) + \lambda\,\delta u_i \frac{\partial}{\partial v_i'}\right) f(\mathbf{r},\mathbf{v}',t) = -\nu(f(\mathbf{r},\mathbf{v}',t) - f_\ell(\mathbf{r},\mathbf{v}',t)) \quad , \tag{4.31}$$

where $\delta\mathbf{u}(\mathbf{r},t)$ is the deviation of the flow velocity from that of the reference state, $\delta\mathbf{u}(\mathbf{r},t) = \mathbf{u}(\mathbf{r},t) - \mathbf{u}_s(\mathbf{r})$. The operator $L(v',a)$ is same as in (4.17). We look for solutions for which all of the space and time dependence occurs through the hydrodynamic fields, $y_\alpha(\mathbf{r},t) \equiv \{n(\mathbf{r},t), T(\mathbf{r},t), \delta\mathbf{u}(\mathbf{r},t)\}$. Such a solution is called a "normal" solution. Near the stationary state, the spatial gradients

of the hydrodynamic variables are small. Since the distribution function is a function of the hydrodynamic variables (i.e. normal solution), we can expand the distribution function with the small gradients as an expansion parameter,

$$f(y_\alpha(\mathbf{r},t),\mathbf{v}') = f^{(0)}(y_\alpha(\mathbf{r},t),\mathbf{v}') + \epsilon f^{(1)}(y_\alpha(\mathbf{r},t),\mathbf{v}') + \cdots, \tag{4.32}$$

where ϵ is a formal parameter representing each spatial gradient relative to the reference state. This is analogous to the Chapman-Enskog method for states near local equilibrium, but here the reference state can be far from equilibrium. In order to determine each $f^{(r)}$ in Eq. (4.31), we need to represent the time derivatives in terms of spatial gradients as well using the hydrodynamic equations. Hence the time derivative also can be expanded in powers of the same ϵ,

$$\frac{\partial}{\partial t} = \frac{\partial^{(0)}}{\partial t} + \epsilon\frac{\partial^{(1)}}{\partial t} + \cdots. \tag{4.33}$$

By putting the expansion (4.32) and (4.33) into Eq.(4.31), equations for each $f^{(r)}$ can be determined. The zeroth order equation is

$$\left(\frac{\partial^{(0)}}{\partial t} - L(v',a) + \lambda\delta\mathbf{u}\cdot\nabla'_{\mathbf{v}}\right) f^{(0)} = -\nu(f^{(0)} - f_\ell), \tag{4.34}$$

and the first order equation is

$$\left(\frac{\partial^{(1)}}{\partial t} + (v'_i + a_{ij}r_j)\frac{\partial}{\partial r_i}\right) f^{(0)} = -\left(\frac{\partial^{(0)}}{\partial t} - L(v',a) + \lambda\delta u_i\frac{\partial}{\partial v'_i} + \nu\right) f^{(1)}. \tag{4.35}$$

First, the zeroth order equation is considered. This equation has the same form as for f_s, (4.15), except that the hydrodynamic fields can have a local space and time dependent parts. Therefore the solution to Eq.(4.34) can be identified as

$$f^{(0)}(\mathbf{r},\mathbf{v}',t) = \nu(\mathbf{r},t)n(\mathbf{r},t)\left(\frac{m}{2\pi k_B T(\mathbf{r},t)}\right)^{3/2}\int_0^\infty d\tau\, \mathrm{e}^{-\nu(\mathbf{r},t)\tau}\mathrm{e}^{3\lambda(\mathbf{r},t)\tau}$$
$$\exp\left(-\frac{m}{2k_B T(\mathbf{r},t)}\mathrm{e}^{2\lambda(\mathbf{r},t)\tau}[\Lambda_{ij}(-\tau)(v_j' - \delta u_j(\mathbf{r},t))]^2\right). \tag{4.36}$$

For consistency, the hydrodynamic variables in $f^{(0)}$ must satisfy the equations

$$\frac{\partial^{(0)}}{\partial t}n = 0, \tag{4.37}$$

$$\frac{\partial^{(0)}T}{\partial t} = 0 \tag{4.38}$$

$$\frac{\partial^{(0)}\delta u_i}{\partial t} + a_{ij}\delta u_j = 0. \tag{4.39}$$

These conditions can be verified easily since they are nothing but the hydrodynamic equations (4.8)-(4.10) at lowest order ϵ,

$$\frac{\partial^{(0)}}{\partial t}n = 0, \tag{4.40}$$

$$\frac{3}{2}nk_B\frac{\partial^{(0)}T}{\partial t} + a_{ij}t_{ij}^{(0)} + 3\lambda p = 0, \tag{4.41}$$

$$\frac{\partial^{(0)}\delta u_i}{\partial t} + a_{ij}\delta u_j = 0, \tag{4.42}$$

where p denotes pressure and $t_{ij}^{(0)}$ is lowest order momentum flux defined by

$$t_{ij}^{(0)} = \int d\mathbf{v}\, m(v_i - u_i)(v_j - u_j) f^{(0)}. \tag{4.43}$$

The extra terms $a_{ij} t_{ij}^{(0)} + 3\lambda p$ in Eq.(4.41) vanish if we calculate the values of $t_{ij}^{(0)}$ from (4.43). The $t_{ij}^{(0)}$ are calculated with a similar integration method used in (4.21a) and they are the same as $t_{s,ij}$ except that now the density and temperature have local space and time dependent parts,

$$t_{xx}^{(0)} = p(\mathbf{r},t) + \frac{4\lambda}{2\lambda+\nu} p(\mathbf{r},t), \tag{4.44a}$$

$$t_{xy}^{(0)} = -\frac{\nu a}{(2\lambda+\nu)^2} p(\mathbf{r},t), \tag{4.44b}$$

$$t_{yy}^{(0)} = p(\mathbf{r},t) - \frac{2\lambda}{2\lambda+\nu} p(\mathbf{r},t), \tag{4.44c}$$

$$t_{zz}^{(0)} = t_{yy}^{(0)}. \tag{4.44d}$$

The extra term in Eq.(4.41) now can be written

$$a t_{xy}^{(0)}(\mathbf{r},t) + 3\lambda p(\mathbf{r},t) = \left(-a \frac{\nu a}{(2\lambda+\nu)^2} + 3\lambda \right) p(\mathbf{r},t) = 0, \tag{4.45}$$

where the relation $3\lambda(2\lambda+\nu)^2 = \nu a^2$ in (4.22) is used. Note that this implies $\lambda = \lambda(n(\mathbf{r},t), T(\mathbf{r},t))$. The conditions for the solution $f^{(0)}$ are now satisfied. The result (4.36) can be viewed as an extension of the stationary solution to its local form, just as the local equilibrium distribution is an extension of the Maxwellian distribution.

The first order distribution function, $f^{(1)}$, can be obtained from Eq.(4.35) since we now know the expression for $f^{(0)}$. The distribution function, $f^{(1)}$ is linear in the hydrodynamic gradients and has the form

$$f^{(1)}(\mathbf{r}, \mathbf{v}', t) = X_{n,i}\frac{\partial n}{\partial r_i} + X_{T,i}\frac{\partial T}{\partial r_i} + X_{u_n,i}\frac{\partial \delta u_n}{\partial r_i}, \tag{4.46}$$

where the $X_{\alpha,i}$ are functions of the velocity to be determined. Substitution of (4.46) into the (4.35) provides a set of coupled equations for these coefficients,

$$\left(\frac{\partial^{(0)}}{\partial t} - L(v', a) + \lambda\, \delta u_i \frac{\partial}{\partial v_i'} + \nu\right) X_{\alpha,k} - a X_{u_x,k}\delta_{\alpha,u_y} = -Y_{\alpha,k}, \tag{4.47}$$

where α denotes n, T, u_x, u_y, and u_z, and i, k represents Cartesian coordinates. The functions $Y_{\alpha,k}$ are given explicitly in terms of $f^{(0)}$, and their detailed form can be found in Appendix E, along with the solution to (4.47). Now the complete normal solution near the uniform shear state is constructed to order ϵ. This is our primary result for describing transport in states near uniform shear flow. It has a form similar to the Chapman-Enskog solution near equilibrium. In both cases the deviation from the reference state is proportional to the hydrodynamic gradients and polynomials in the velocity. Here, however, the reference state is not Gaussian and depends on the shear rate. In addition, the coefficients, $X_{\alpha,k}$ also have a strong dependence on shear rates. Therefore even though this normal solution is valid for small spatial gradients from the reference, it can be applied to any finite shear rate.

4.3 Hydrodynamic Equations

The BGK-Boltzmann equation gives the hydrodynamic equations by integrating the equations with summational invariants. They are Eqs.(4.8)-(4.10). These are an exact set of equations, but incomplete. Once the moment and heat fluxes are specified as functionals of the hydrodynamic variables, a closed set of equations may be obtained. At the low density near equilibrium, they are expressed by a "Newton's viscosity law" for momentum flux and "Fourier's heat law" for heat flux. The hydrodynamic equations combined with these fluxes are called the Navier-Stokes equations. Far from equilibrium state, no specific constitute equations are known in general. However by using our normal solution from section 4.2, we can calculate these fluxes for the special case of a system near uniform shear flow. The fluxes can be written with two terms,

$$t_{ij} = t_{ij}^{(0)} + \epsilon t_{ij}^{(1)}, \tag{4.48}$$

$$q_i = q_i^{(0)} + \epsilon q_i^{(1)}, \tag{4.49}$$

where

$$t_{ij}^{(r)} = \int d\mathbf{v} m(v_i - u_i)(v_j - u_j) f^{(r)}, \tag{4.50}$$

$$\mathbf{q}^{(r)} = \int d\mathbf{v} \frac{1}{2} m(\mathbf{v} - \mathbf{u})^2 (\mathbf{v} - \mathbf{u}) f^{(r)}. \tag{4.51}$$

$t_{ij}^{(0)}$ and $q_i^{(0)}$ represent the transport properties at the local reference state and they are already calculated in the previous section. The second terms, $t_{ij}^{(1)}$ and $q_i^{(1)}$ describe gradients near the reference state and can be calculated from the

definition (4.50) and (4.51) by using $f^{(1)}$. They are written in terms of deviations in the hydrodynamic variables from the reference state,

$$t_{ij}^{(1)} = \gamma_{lk}^{ij} \frac{\partial \delta u_l}{\partial r_k}, \tag{4.52}$$

and

$$q_i^{(1)} = \xi_{T,j}^{i} \frac{\partial T}{\partial r_j} + \xi_{n,j}^{i} \frac{\partial n}{\partial r_j}. \tag{4.53}$$

The coefficients of the gradients are generalized transport coefficients given by

$$\gamma_{lk}^{ij} = \int d\mathbf{v} m(v_i - u_j)(v_j - u_j) X_{u_l,k}, \tag{4.54}$$

$$\xi_{\alpha,j}^{i} = \int d\mathbf{v} \frac{1}{2} m(v - u)^2 (v_i - u_i) X_{\alpha,j}, \tag{4.55}$$

where α denotes n and T and i, j, k, and l represent x, y, z. Their detailed calculation and resultant functions of the shear rate can be found in Appendix F. There are many new transport coefficients which do not exist for states near equilibrium due in part to the anisotropy of the reference state. Eqs.(4.24)-(4.26) show the transport coefficients at the reference state. The heat flux was zero at the state because of the definition of the uniform shear flow (uniform temperature). Now let us examine how the thermal conductivity changes near the reference state under the shear effect. The thermal conductivity is defined as the coefficients of the temperature gradients, so $\xi_{T,j}^{i}$ in (4.53) can be identified as a generalized thermal conductivity tensor. This is due to the anisotropy of the reference state. The diagonal parts, λ_{jj} are shown in Figure 4.2 as a function of shear rate.

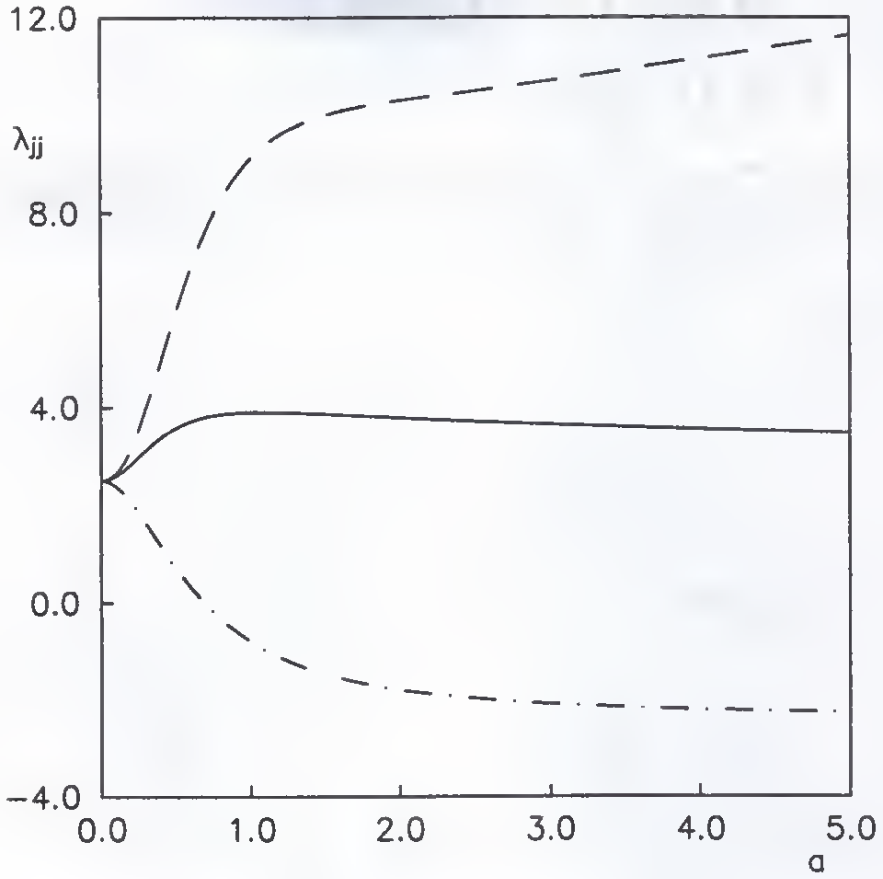

Figure 4.2: The diagonal parts of the generalized thermal conductivity, $\lambda_{jj}(a)$ are shown as a function of a. The solid line is for $j = y$, the dashed line is for $j = x$, and the dash-dot line is for $j = z$. λ_{jj} is in unit of $k_B p_s/m\nu$ and a is in unit of ν.

With all the shear dependent generalized transport coefficients known, the new constitute equations are completed, and a corresponding the set of closed hydrodynamic equations is obtained. These equations are again valid to second order in spatial gradients relative to the reference state, but there is no restriction on the value of shear rate (in other words, there is no restriction for how far the

reference state should be from equilibrium state). Finally, the hydrodynamic equations are

$$(D_t + \delta\mathbf{u}\cdot\nabla)n + n\nabla\cdot\delta\mathbf{u} = 0, \tag{4.56}$$

$$\frac{3}{2}nk_B(D_t + \delta\mathbf{u}\cdot\nabla)T + a_{ij}\gamma^{ij}_{lm}\frac{\partial\delta u_l}{\partial r_m} + \frac{\partial\delta u_i}{\partial r_j}[t^{(0)}_{ij} + \gamma^{ij}_{lm}\frac{\partial\delta u_l}{\partial r_m}] + \frac{\partial}{\partial r_i}[\xi^i_{n,j}\frac{\partial n}{\partial r_j} + \xi^i_{T,j}\frac{\partial T}{\partial r_j}] = 0, \tag{4.57}$$

$$(D_t + \delta\mathbf{u}\cdot\nabla)\delta u_k + \rho^{-1}\frac{\partial}{\partial r_i}[t^{(0)}_{ik} + \gamma^{ik}_{lm}\frac{\partial\delta u_l}{\partial r_m}] + a_{kj}\delta u_j = 0, \tag{4.58}$$

where $D_t = \frac{\partial}{\partial t} + a_{ij}r_j\frac{\partial}{\partial r_i}$. The density equation is the usual Euler equation. At the local stationary state (the reference state), the temperature is constant due to the thermostat (see Eq.(4.41)). However, near the uniform shear state the temperature changes due to the spatial gradients of the hydrodynamic variables. The momentum flux from the reference state, $t^{(0)}_{ij}$, can be divided into reversible and the irreversible parts as in Eq.(4.44a), where the pressure gives the usual Euler contribution.

CHAPTER 5
TWO TIME CORRELATION EQUATION

The kinetic model equation for the two time phase space correlation function is given by Eq.(3.38). In this chapter, this two time correlation function is considered for uniform shear flow. The equation for the two time correlation function has the same structure as that for the distribution function linearized around the reference state. Hence the analysis of the two time correlation function in the reference state provides a way of studying both transport properties for states near uniform shear flow and the stability of the reference state (a generalization of Onsager's assumption on the regression of fluctuations [32,33]). Similarly, the dynamics for fluctuations of the hydrodynamic fields in the reference state is the same as the linearized hydrodynamic equations of the previous chapter for small perturbations. To study the transport properties and stability of the states near uniform shear flow, we solve the dispersion relations from these linearized hydrodynamic equations and obtain the five modes which govern the long time, large wavelength dynamics of the system. For any finite shear rate and sufficiently long wavelength, we find that a pair of propagating modes are unstable for this flow. This new instability is compared with a Monte Carlo simulation of the distribution function using the Bird method [20] and shows excellent agreement. To address the question that this instability might be an anomaly of the BGK-kinetic model, we study the stability at small shear rates directly from the

usual Navier-Stokes equations for the hard sphere case at both low and high densities. The analysis shows the long wavelength instability again. These results indicate that this instability is not a consequence of the assumptions behind the hydrodynamic calculation or use of the low density BGK-kinetic model.

5.1 Linearized Hydrodynamic Equations

In Chapter 3, we derived the kinetic model for the equation of two time phase correlation function, (3.38). The formal solution ($t' = 0$) to the equation is written in Fourier representation,

$$\tilde{C}(\mathbf{k}, \mathbf{v}, t; \mathbf{k}', \mathbf{v}', 0) = e^{-t\tilde{\mathcal{L}}(\mathbf{k},\mathbf{v})}\tilde{C}(\mathbf{k}, \mathbf{v}, 0; \mathbf{k}', \mathbf{v}', 0), \tag{5.1}$$

where the operator $\mathcal{L}$ is defined in Eq.(3.40). The time evolution operator in the two time correlation equation is the same as that for the BGK-Boltzmann equation linearized around the reference state, $\delta\tilde{f} = \widetilde{f - f_s}$,

$$\delta\tilde{f}(\mathbf{k}, \mathbf{v}, t) = e^{-t\tilde{\mathcal{L}}(\mathbf{k},\mathbf{v})}\delta\tilde{f}(\mathbf{k}, \mathbf{v}, 0). \tag{5.2}$$

Hence as far as the dynamics is concerned, the two time correlation function and linearized distribution function have same time dependence. This is an example of a nonequilibrium fluctuation-dissipation relation. The two time correlation function describes the dynamics of spontaneous fluctuations in the reference state, but it also represents the linear response function for small perturbations of the

reference state. Consequently by analyzing fluctuations in the reference state, we can study how a disturbance of that state decays or grows in time.

While it is possible to study directly the spectrum of $\mathcal{L}$ and consequently all possible relaxation modes, here we focus instead on the hydrodynamic spectrum which is expected to dominate for long times. The two time matrix of the hydrodynamic correlation function is defined by velocity integration with $\psi_\alpha = \{1, \mathbf{v}, v^2\}$ (see Eq.(3.10)),

$$\tilde{C}_{\alpha\beta}(\mathbf{k}, t; \mathbf{k}', 0) \equiv \int d\mathbf{v} d\mathbf{v}' \, \psi_\alpha(v) \psi_\beta(v') \mathrm{e}^{-t\tilde{\mathcal{L}}(\mathbf{k},\mathbf{v})} \tilde{C}(\mathbf{k}, \mathbf{v}, 0; \mathbf{k}', \mathbf{v}', 0) \tag{5.3}$$

$$= \int d\mathbf{v} \, \psi_\alpha(v) \mathrm{e}^{-t\tilde{\mathcal{L}}(\mathbf{k},\mathbf{v})} \int d\mathbf{v}' \, \psi_\beta(v') \tilde{C}(\mathbf{k}, \mathbf{v}, 0; \mathbf{k}', \mathbf{v}', 0), \tag{5.4}$$

and similarly the Fourier transformation of the linearized hydrodynamic variables, $\delta\tilde{y}_\alpha$, for deviations from the reference state are given by

$$\delta\tilde{y}_\alpha(\mathbf{k}, t) = \int d\mathbf{v} \psi_\alpha(v) \mathrm{e}^{-t\tilde{\mathcal{L}}(\mathbf{k},v)} \delta\tilde{f}(\mathbf{k}, \mathbf{v}, 0). \tag{5.5}$$

Thus $\tilde{C}_{\alpha\beta}(\mathbf{k}, t; \mathbf{k}', 0)$ are the response functions for hydrodynamic perturbations. The advantage of this is that we can use the hydrodynamic equations (4.56)-(4.58) which were derived in the last chapter, to construct the equations for both $\tilde{C}_{\alpha\beta}(t)$ and $\delta\tilde{y}_\alpha(t)$.

The deviations of the hydrodynamic variables from uniform shear flow are defined by

$$\delta n(\mathbf{r},t) = n(\mathbf{r},t) - n_s,\ \ \delta T(\mathbf{r},t) = T(\mathbf{r},t) - T_s,\ \ \delta \mathbf{u}(\mathbf{r},t) = \mathbf{u}(\mathbf{r},t). \tag{5.6}$$

Substitution of these variables into the hydrodynamic equations (4.56)-(4.58), and retaining only linear terms gives

$$D_t\,\delta n + n_s \nabla \cdot \delta \mathbf{u} = 0, \tag{5.7}$$

$$D_t\,\delta T + \frac{2}{3n_s k_B}\left(a\gamma^{xy}_{ij,s} + t^{(0)}_{ij,s}\right)\frac{\partial \delta u_i}{\partial r_j} + \frac{2}{3n_s k_B}\left[\xi^i_{nj,s}\frac{\partial^2 \delta n}{\partial r_i \partial r_j} + \xi^i_{Tj,s}\frac{\partial^2 \delta T}{\partial r_i \partial r_j}\right] = 0, \tag{5.8}$$

$$D_t\,\delta u_k + \rho_s^{-1}\left[\left(\frac{\partial t^{(0)}_{ik}}{\partial n}\right)_s \frac{\partial \delta n}{\partial r_i} + \left(\frac{\partial t^{(0)}_{ik}}{\partial T}\right)_s \frac{\partial \delta T}{\partial r_i} + \gamma^{ik}_{lm,s}\frac{\partial^2 \delta u_l}{\partial r_i \partial r_m}\right] + a_{kj}\delta u_j = 0, \tag{5.9}$$

where s denotes a stationary value. These equations can be written for dimensionless hydrodynamic variables, $\delta\tilde{y}_\alpha$, in Fourier representation form for convenience,

$$\left(\frac{\partial}{\partial t} + a_{ij}k_i\frac{\partial}{\partial k_j}\right)\delta\tilde{y}_\alpha + (A_{\alpha\beta} - i\sum_j k_j B_{\alpha\beta,j} - \sum_{j,l} k_j k_l D_{\alpha\beta,jl})\delta\tilde{y}_\beta = 0, \tag{5.10}$$

where $\delta\tilde{y}_\alpha$ is

$$\delta\tilde{y}_\alpha = \left\{\frac{\delta\tilde{n}}{n_s}, \sqrt{\frac{3}{2}}\frac{\delta\tilde{T}}{T_s}, \sqrt{\frac{m}{k_B T_s}}\delta\tilde{\mathbf{u}}\right\}, \tag{5.11}$$

and j, l denote x, y, z. The three matrices $A_{\alpha\beta}, B_{\alpha\beta}, D_{\alpha\beta}$ are

$$A_{\alpha\beta} = \begin{pmatrix} 0\,0\,0\,0\,0 \\ 0\,0\,0\,0\,0 \\ 0\,0\,0\,a\,0 \\ 0\,0\,0\,0\,0 \\ 0\,0\,0\,0\,0 \end{pmatrix} \tag{5.12}$$

$$B_{\alpha\beta j} = \sqrt{\frac{k_B T_s}{m}} \begin{pmatrix} 0 & 0 & \delta_{jx} & \delta_{jy} & \delta_{jz} \\ 0 & 0 & B_{2xj} & B_{2yj} & B_{2zj} \\ \frac{n}{p_s}\left(\frac{\partial t^{(0)}_{jx}}{\partial n}\right)_s & \sqrt{\frac{2}{3}}\frac{T_s}{p_s}\left(\frac{\partial t^{(0)}_{jx}}{\partial T}\right)_s & 0 & 0 & 0 \\ \frac{n}{p_s}\left(\frac{\partial t^{(0)}_{jy}}{\partial n}\right)_s & \sqrt{\frac{2}{3}}\frac{T_s}{p_s}\left(\frac{\partial t^{(0)}_{jy}}{\partial T}\right)_s & 0 & 0 & 0 \\ \frac{n}{p_s}\left(\frac{\partial t^{(0)}_{js}}{\partial n}\right)_s & \sqrt{\frac{2}{3}}\frac{T_s}{p_s}\left(\frac{\partial t^{(0)}_{jz}}{\partial T}\right)_s & 0 & 0 & 0, \end{pmatrix} \tag{5.13}$$

where $B_{2ij} = \sqrt{\frac{2}{3}}\frac{1}{p_s}(a\gamma^{xy}_{ij,s} + t^{(0)}_{ij,s})$. The matrix $D_{\alpha\beta}$ is

$$D_{\alpha\beta jl} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ \sqrt{\frac{2}{3}}\frac{n_s}{p_s}\xi^j_{nl,s} & \frac{2}{3}\frac{T_s}{p_s}\xi^j_{Tl,s} & 0 & 0 & 0 \\ 0 & 0 & \rho^{-1}\gamma^{jx}_{xl,s} & \rho^{-1}\gamma^{jx}_{yl,s} & \rho^{-1}\gamma^{jx}_{zl,s} \\ 0 & 0 & \rho^{-1}\gamma^{jy}_{xl,s} & \rho^{-1}\gamma^{jy}_{yl,s} & \rho^{-1}\gamma^{jy}_{zl,s} \\ 0 & 0 & \rho^{-1}\gamma^{jz}_{xl,s} & \rho^{-1}\gamma^{jz}_{yl,s} & \rho^{-1}\gamma^{jz}_{zl,s} \end{pmatrix}, \tag{5.14}$$

where j, l represents Cartesian coordinates. The homogeneous solution to

equations (5.10) can be calculated easily by putting $\mathbf{k} = 0$,

$$\delta n(t) = \delta n(0), \tag{5.15}$$

$$\delta T(t) = \delta T(0), \tag{5.16}$$

$$\delta u_x(t) = \delta u_x(0) - at\delta u_y(0), \tag{5.17}$$

$$\delta u_y(t) = \delta u_y(0), \tag{5.18}$$

$$\delta u_z(t) = \delta u_z(0). \tag{5.19}$$

These are the expected results from Eqs.(4.37)-(4.39). Thus the homogeneous state is unstable to perturbations in $\delta\widetilde{u}_y$, leading to unbounded linear change in time. It is expected that this should be controlled at finite k by exponential damping factors, $e^{-\alpha k^2 t}$ (α is a damping constant). This question is addressed in the next section.

5.2 Hydrodynamic Modes

For the inhomogeneous case, to simplify the analysis we allow the perturbation only along the velocity gradient direction, i.e. $k_x = k_z = 0$. In this case the linear hydrodynamic equations become simpler (i.e. $D_t \to \partial_t$), and the hydrodynamic modes can be calculated directly from dispersion relations. The linearized hydrodynamic equations became

$$\frac{\partial}{\partial t}\delta\widetilde{y}_\alpha + F_{\alpha\beta}\delta\widetilde{y}_\beta = 0, \tag{5.20}$$

where $F_{\alpha\beta} = A_{\alpha\beta} - ik_y B'_{\alpha\beta} - k_y^2 D'_{\alpha\beta}$. The prime means the case of $k_x = k_z = 0$. Matrices B', D' are simpler and they are given by

$$B'_{\alpha\beta} = \sqrt{\frac{k_B T_s}{m}} \begin{pmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & B_{2xy} & B_{2yy} & 0 \\ \frac{n_s}{p_s}\left(\frac{\partial t_{yx}^{(0)}}{\partial n}\right)_s & \sqrt{\frac{2}{3}}\frac{T_s}{p_s}\left(\frac{\partial t_{yx}^{(0)}}{\partial T}\right)_s & 0 & 0 & 0 \\ \frac{n_s}{p_s}\left(\frac{\partial t_{yy}^{(0)}}{\partial n}\right)_s & \sqrt{\frac{2}{3}}\frac{T_s}{p_s}\left(\frac{\partial t_{yy}^{(0)}}{\partial T}\right)_s & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \tag{5.21}$$

$$D'_{\alpha\beta} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ \sqrt{\frac{2}{3}}\frac{n_s}{p_s}\xi_{ny,s}^y & \frac{2}{3}\frac{T_s}{p_s}\xi_{Ty,s}^y & 0 & 0 & 0 \\ 0 & 0 & \rho_s^{-1}\gamma_{xy,s}^{yx} & \rho_s^{-1}\gamma_{yy,s}^{yx} & 0 \\ 0 & 0 & \rho_s^{-1}\gamma_{xy,s}^{yy} & \rho_s^{-1}\gamma_{yy,s}^{yy} & 0 \\ 0 & 0 & 0 & 0 & \rho_s^{-1}\gamma_{zy,s}^{yz} \end{pmatrix}. \tag{5.22}$$

Equation (5.20) can be solved by Laplace transformation,

$$(zI + F)\widehat{\delta y}(\mathbf{k}, z) = \delta\tilde{y}(\mathbf{k}, t = 0), \tag{5.23}$$

where

$$\widehat{\delta y}(\mathbf{k}, z) = \int_0^\infty dt\, e^{-tz}\delta\tilde{y}(\mathbf{k}, t). \tag{5.24}$$

Then, the $\widehat{\delta y}(\mathbf{k}, z)$ is

$$\widehat{\delta y}_\alpha(\mathbf{k}, z) = K_{\alpha\beta}^{-1}\,\delta\tilde{y}_\beta(\mathbf{k}, t = 0) \tag{5.25}$$

where

$$K_{\alpha\beta}(\mathbf{k}, z) \equiv [zI + F]_{\alpha\beta}. \tag{5.26}$$

The determinant of the matrix K gives the five simple hydrodynamic poles that determine the dominant dynamics of the $\delta y_\alpha(\mathbf{k}, t)$ at large t and small k. At equilibrium (zero shear rate), the matrix $K_{\alpha\beta}$ becomes identical to the matrix $B_{\alpha\beta}$ in (3.60) and they give the expected five hydrodynamic modes; two sound modes, a heat mode and two shear modes which were already discussed in the first example of section 3.4. For finite shear rate, the determinant is complicated and it is very difficult to find the dispersion relations analytically . The best way to understand the dispersion relations for finite a is to calculate each pole for a given value of a. For convenience, we use dimensionless variables for k, a in units of inverse mean free path, inverse mean free time respectively. Also since the last element in δy_α is decoupled from other elements in the matrix K, the dispersion relations are only considered for four hydrodynamic modes. They are obtained from the equation

$$\det(K_{\alpha\beta}(\mathbf{k}, a, z)) \equiv (z - z_1(\mathbf{k}, a))(z - z_2(\mathbf{k}, a))(z - z_3(\mathbf{k}, a))(z - z_4(\mathbf{k}, a)) = 0. \tag{5.27}$$

First, when the shear rate is 0.1,

$$z_1 \xrightarrow{k\to 0} (0.093 - 0.16\,i)\,k^{2/3} + (-0.75 - 1.3\,i)\,k^{4/3} - 0.5\,k^2 \tag{5.28}$$

$$z_2 = z_1^* \tag{5.29}$$

$$z_3 \xrightarrow{k\to 0} -0.49\,k^2, \tag{5.30}$$

$$z_4 \xrightarrow{k\to 0} -0.19\,k^{2/3} + 1.5\,k^{4/3} - 0.5\,k^2. \tag{5.31}$$

Notice that the real values of z_1 and z_2 are positive, which means that the hydrodynamic modes are growing in time instead of decaying back to the reference state. Also most modes are not analytic functions of k, so it is not possible to identify them simply in terms of the equilibrium hydrodynamic modes. The system is unstable for the chosen value of the shear rate at asymptotically small k. Now let us do a numerical calculation at large k ($k = 0.2$) with the same value of the shear rate to see what happens to the unstable modes,

$$z_1 = (-0.016 - 0.18\,i) \tag{5.32}$$

$$z_2 = z_1^* \tag{5.33}$$

$$z_3 = -0.02 \tag{5.34}$$

$$z_4 = -0.028 \tag{5.35}$$

These unstable modes become stable at this large k. From this analysis, we may speculate that there are separate domains for stable and unstable dynamics in the wavevector and shear rate plane. The figure 5.1 shows the critical line dividing the stable (above) and unstable (below) regions in the k - a plane.

This instability is an obstacle in the study of the dynamics of the hydrodynamic modes. According to the figure 5.1, for any nonzero shear rate and small k, there is always an instability. It seems that the dynamics become stable when the wavevector $kv_0 > a$, where v_0 is a thermal velocity, defined by $\sqrt{2k_BT/m}$. To study the stable dynamics of the hydrodynamic modes, we introduce a new

dimensionless variable, $x = kv_0/a$, in the matrix F of Eq.(5.20). This new variable has a minimum number which depends on the choice of the shear rate value. For example $x > 0.75$ for $a < 0.3\nu$ to be in the stable region. The numbers were

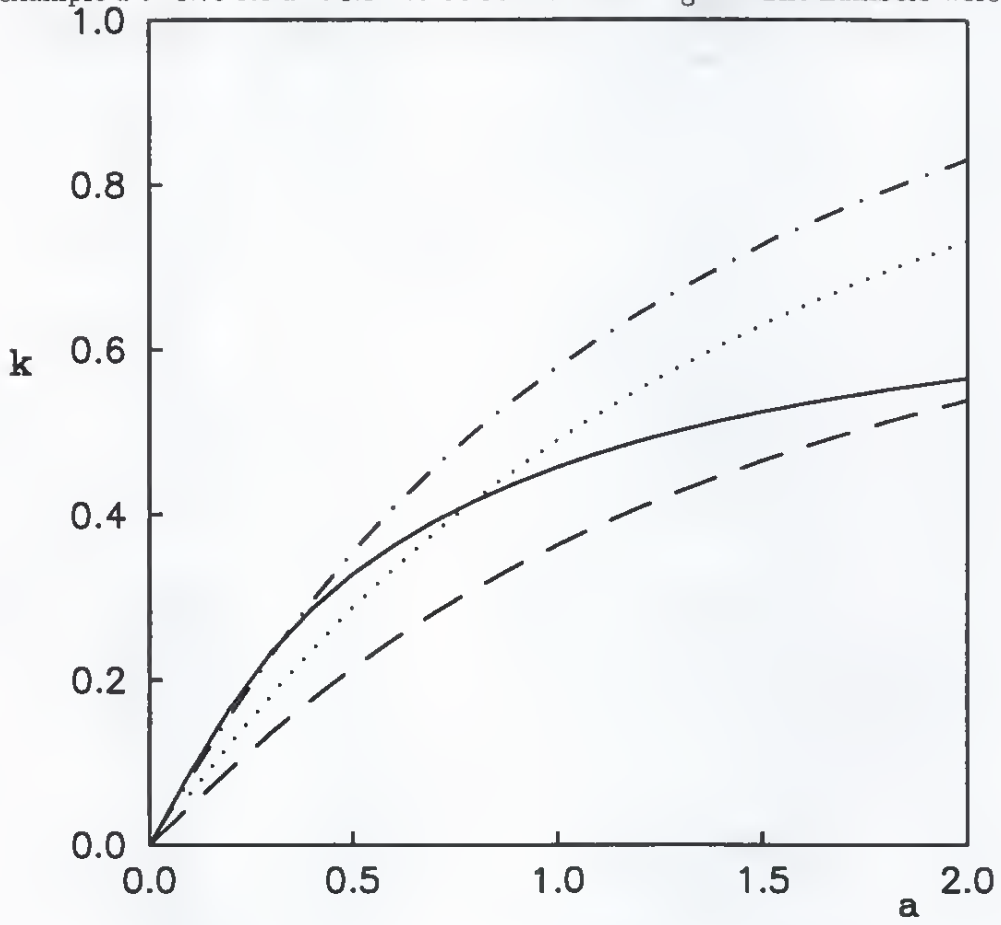

Figure 5.1: Critical lines for stability are shown. The BGK-kinetic model gives the solid line and the other three lines are from Navier-Stokes order for different densities. Dashed-dot line is for $n^* = 0$, dotted curve is for $n^* = 0.2$ and dashed curve is for $n^* = 0.4$. All are in units of the mean free path and mean free time.

determined from figure 5.1. Therefore the x is not a small variable. Now all the shear rates in the matrix F may be replaced by kv_0/x and the matrix F becomes

a function of k and x. The Eq.(5.20) now can be calculated by the perturbation method with small k at fixed x and the solution, $\delta y_\alpha(k,t)$, will show the dynamics in the stable domain for the hydrodynamic modes. The eigenvalues of matrix F are calculated from $\det(F - sI) = 0$, where s are eigenvalues and I is an Identity matrix. Also the corresponding eigenvectors, ζ, can be obtained

$$F(k,x)\,\zeta^{(i)} = s_i(k,x)\,\zeta^{(i)}. \tag{5.36}$$

For the convenience of the calculation, the dimensionless variables are used again.

$$k^* = kv_0/\nu, \quad a^* = a/\nu, \quad s^* = s/\nu. \tag{5.37}$$

The eigenvalue problem is solved for 2-dimensions. Then the dimensionless eigenvalues up to order k^2 are

$$s_1^* = \frac{k^{*2}}{2}, \tag{5.38}$$

$$s_2^* = \frac{k^{*2}}{2} + \frac{2\,k^{*2}}{5\,x^2}, \tag{5.39}$$

$$s_3^* = -i\sqrt{\frac{5}{6}}k^* + \left(\frac{1}{2} - \frac{1}{5\,x^2}\right)k^{*2}, \tag{5.40}$$

$$s_4^* = i\sqrt{\frac{5}{6}}k^* + \left(\frac{1}{2} - \frac{1}{5\,x^2}\right)k^{*2}. \tag{5.41}$$

Notice that in this perturbation x is fixed at larger than $\sqrt{\frac{2}{5}}$. These eigenvalues are now analytic functions of k in the stable region and it is possible to recognize them as familiar sound modes, heat modes and a shear mode. The corresponding

eigenvectors are

$$\zeta^{(1)} = \left(-\sqrt{\frac{2}{5}}, \sqrt{\frac{3}{5}}, -\frac{i}{\sqrt{5}x}, 0\right), \tag{5.42}$$

$$\zeta^{(2)} = \left(-\sqrt{\frac{2}{5}}, \sqrt{\frac{3}{5}}, -\frac{2i}{\sqrt{5}x}, 0\right) \tag{5.43}$$

$$\zeta^{(3)} = \left(\sqrt{\frac{3}{5}}, \sqrt{\frac{2}{5}}, \sqrt{\frac{6}{5}}\frac{i}{x}, 1\right), \tag{5.44}$$

$$\zeta^{(4)} = \left(\sqrt{\frac{3}{5}}, \sqrt{\frac{2}{5}}, \sqrt{\frac{6}{5}}\frac{i}{x}, -1\right). \tag{5.45}$$

The associated biorthogonal set is denoted by $\{\eta^{(i)}\}$,

$$\sum_{\alpha=1}^{4} \zeta_\alpha^{(i)} \eta_\alpha^{(j)} = \delta_{ij}, \tag{5.46}$$

and they are

$$\eta^{(1)} = (-\sqrt{10}, 0, -i\sqrt{5}x, 0), \tag{5.47}$$

$$\eta^{(2)} = \left(\sqrt{\frac{5}{2}} + \frac{3}{\sqrt{10}}, \sqrt{\frac{3}{5}}, i\sqrt{5}x, 0\right), \tag{5.48}$$

$$\eta^{(3)} = \left(\frac{1}{2}\sqrt{\frac{3}{5}}, \frac{1}{\sqrt{10}}, 0, \frac{1}{2}\right), \tag{5.49}$$

$$\eta^{(4)} = \left(\frac{1}{2}\sqrt{\frac{3}{5}}, \frac{1}{\sqrt{10}}, 0, -\frac{1}{2}\right). \tag{5.50}$$

The linearized hydrodynamic variables, $\delta\tilde{y}_\alpha$ can be expressed in terms of these

eigenvalues and eigenfunctions,

$$\delta\widetilde{y}_\alpha(\mathbf{k},t) = \sum_i \mathrm{e}^{-ts_i(\mathbf{k},x)}\zeta_\alpha^{(i)}(\mathbf{k},x)\eta_\beta^{(i)}(\mathbf{k},x)\delta\widetilde{y}_\beta(\mathbf{k},0). \tag{5.51}$$

It is also possible to give the two time hydrodynamic correlation function, Eq.(5.4), with these eigenvalues and eigenvectors because they share the same time evolution operator,

$$\widetilde{C}_{\alpha\beta}(\mathbf{k},t;\mathbf{k}',0) = \sum_{i=1}^{4} \mathrm{e}^{-s_i(k,x)t}\zeta_\alpha^{(i)}(\mathbf{k},x)\eta_\sigma^{(i)}(\mathbf{k},x)\widetilde{C}_{\sigma\beta}(\mathbf{k},0;\mathbf{k}',0), \tag{5.52}$$

where the $\widetilde{C}_{\alpha\beta}(\mathbf{k},0;\mathbf{k}',0)$ is an equal time correlation function. The discussion of it will be deferred to the next chapter. The two time hydrodynamic correlation function can be used to calculate the dynamic structure factor, $S(\mathbf{k},w)$. It describes the density fluctuation that can be measured in light scattering experiment,

$$S(\mathbf{k},w) = \int_{-\infty}^{\infty} dt\,\Theta(\mathbf{k}-\mathbf{k}_{min})\Theta(\mathbf{k}'-\mathbf{k}'_{min})\widetilde{C}_{nn}(\mathbf{k},t;\mathbf{k}',0)\mathrm{e}^{iwt}, \tag{5.53}$$

where the Θ function restricts the spatial regions because of the instabilities. The expression can be written to identify the modified Brillouin and Rayleigh peaks,

$$S(\mathbf{k},w) = S_R(\mathbf{k},w) + S_B(\mathbf{k},w) + S_B(\mathbf{k},-w), \tag{5.54}$$

with

$$S_R(\mathbf{k},w) = 2\,\mathrm{Re}[-iw + \frac{k^2}{\beta m\nu}]^{-1} 2\,\tilde{C}_{11}(\mathbf{k},a) + 2\,\mathrm{Re}[-iw + \frac{k^2}{\beta m\nu} + \frac{2a^2}{5\nu}]^{-1}(\frac{8}{5}\,\tilde{C}_{11}(\mathbf{k},a) + \frac{\sqrt{6}}{5}\,\tilde{C}_{21}(\mathbf{k},a))), \quad (5.55)$$

$$S_B(\mathbf{k},w) = 2\,\mathrm{Re}[-i(w+c_0k) + \frac{k^2}{\beta m\nu} - \frac{a^2}{5\nu}]^{-1}(\frac{3}{10}\tilde{C}_{11}(\mathbf{k},a) + \frac{\sqrt{6}}{10}\tilde{C}_{21}(\mathbf{k},a)), \quad (5.56)$$

where $\beta = 1/k_BT$ and $\tilde{C}_{\alpha\beta}(\mathbf{k},a)$ are equal time correlation functions. Also c_0 is a sound velocity.

Now let us examine more closely the instability [45] we found. First, to illustrate how the unstable modes behave in time, Eq.(5.20) is solved for given numerical values of k and a, which were chosen from the unstable region in figure 5.1. The calculations are done with the values of $k^* = kl_{mfp} = 0.1$ and $a^* = a/\nu = 0.5$ and for initial deviations, $\delta\tilde{y}(\mathbf{k}, t=0) = \{0, 0, -0.3y_{40}, y_{40}\}$ are chosen and y_{40} is constant. The detailed calculation is given in Appendix G. The calculation is done for 2-dimensions because the z-component of the velocity deviation, δu_z is decoupled from Eq.(5.20). This is easily solvable,

$$\delta\tilde{u}_z(\mathbf{k},t) = e^{-t\rho_s^{-1}\gamma^{yz}_{zy,s}}\delta\tilde{u}_z(\mathbf{k},0) \quad (5.57)$$

$$= \mathrm{e}^{-t\frac{k_BT}{m}\frac{2\lambda}{(2\lambda+\nu)^2}}\delta\tilde{u}_z(\mathbf{k},0). \quad (5.58)$$

Now the remaining hydrodynamic variables are

$$\delta\tilde{y}_4(t^*) = y_{40}[0.17002\mathrm{e}^{-0.0569012\,t^*} - 0.00139119\mathrm{e}^{-0.00320425\,t^*} (0.83128\cos(0.103845\,t^*) - 0.111384\sin(0.103845\,t^*))\mathrm{e}^{0.020532\,t^*}], \tag{5.59}$$

$$\delta\tilde{y}_3(t^*) = y_{40}[1.41137\mathrm{e}^{-0.0569012\,t^*} - 0.0730989\mathrm{e}^{-0.00320425\,t^*} +(-1.63828\cos(0.103845\,t^*) - 3.68154\sin(0.103845\,t^*))\mathrm{e}^{0.020532\,t^*}], \tag{5.60}$$

$$\delta\tilde{y}_2(t^*) = iy_{40}[0.435579\mathrm{e}^{-0.0569012\,t^*} - 0.0422361\mathrm{e}^{-0.0032425\,t^*} +(-0.393344\cos(0.103845\,t^*) + 1.09344\sin(0.103845\,t^*))\mathrm{e}^{0.020532\,t^*}], \tag{5.61}$$

$$\delta\tilde{y}_1(t^*) = iy_{40}[-0.211397\mathrm{e}^{-0.0569012\,t^*} + 0.0307004\mathrm{e}^{-0.0032425\,t^*} (0.180697\cos(0.103845\,t^*) + 0.530312\sin(0.103845\,t^*))\mathrm{e}^{0.020532\,t^*}], \tag{5.62}$$

where t^* is time in units of ν. Figure 5.2 shows the results for $\delta\tilde{u}_x(t^*)$ and $\delta\tilde{u}_y(t^*)$ as function of time. It is seen that there is an unstable propagating mode of increasing amplitude of the maxima and minima. This is compared with a Monte Carlo simulation of the BGK-kinetic equation using extended Bird method [46] by José M. Montanero and Andrés Santos. This computer simulation is done without any detailed hydrodynamic equation information. The excellent agreement shows that the instability is not a result of the assumptions behind the

hydrodynamic equations. Even though the computer simulation shows a good agreement, it brings up the possibility that the instability might be an anomaly of the BGK-kinetic model, so it might not be a physical property. To answer

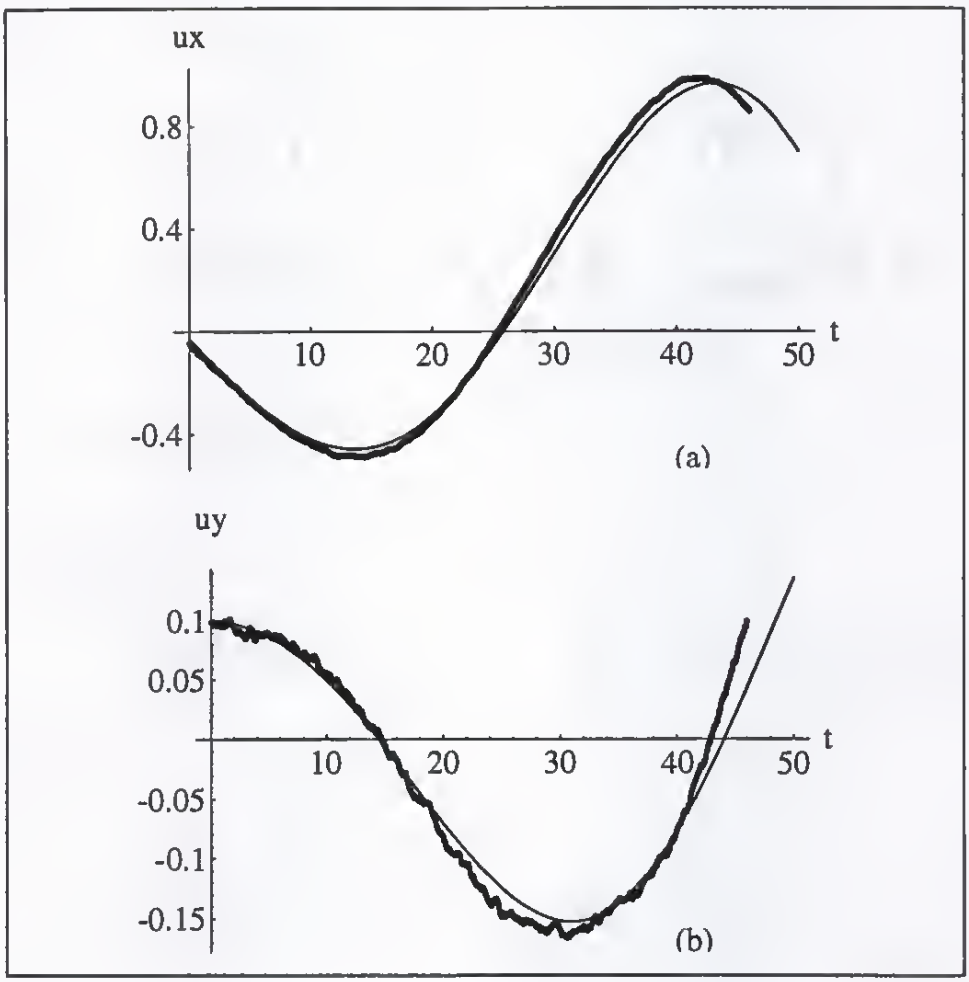

Figure 5.2: Time evolution of (a)$\delta\tilde{u}_x(t^*)$ and (b) $\delta\tilde{u}_y(t^*)$ for $a* = 0.5$ and $k* = 0.1$.

this question, we have calculated the dispersion relations on Navier-Stokes order without kinetic models. The Navier-Stokes order means that the gradients of the

thermodynamic variables are very small including the shear rate as well, so the heat and momentum fluxes are specified by Fourier's law and Newton's viscosity law. We consider this time a fluid of hard spheres, not a Maxwell molecules case, in order to find the effect of the density dependence on the instability. The equation of state for hard spheres is calculated using Enskog kinetic theory and Percus-Yevick approximation and the transport coefficients are estimated from the Chapman-Enskog method [47–49]. The linearized hydrodynamic equations for y_α are

$$\left(\frac{\partial}{\partial t} + A_N - ikB_N + k^2 D_N\right)\delta\tilde{y}_\alpha = 0, \tag{5.63}$$

where "N" denotes Navier-Stokes order and $k = k_y$. The matrices are

$$A_N = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & a \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{5.64}$$

$$B_N = \sqrt{\frac{k_B T}{m}} \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -\sqrt{\frac{2}{3}}\frac{a}{p_0} 2\eta_s & \sqrt{\frac{2}{3}} \\ -\frac{a}{p_0} n_s \frac{\partial \eta}{\partial n} & -\sqrt{\frac{2}{3}}\frac{a}{p_0} T_s \frac{\partial \eta}{\partial T} & 0 & 0 \\ \frac{n_s}{p_0}\frac{\partial p}{\partial n} & \sqrt{\frac{2}{3}}\frac{T_s}{p_0}\frac{\partial p}{\partial T} & 0 & 0 \end{pmatrix}, \tag{5.65}$$

where ϵ is the internal energy, η is the shear viscosity and p_0 is the pressure of

ideal gas. Finally the matrix D_N is

$$D_N = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{2}{3}\frac{\kappa}{n_s k_B} & 0 & 0 \\ 0 & 0 & \frac{\eta}{\rho} & 0 \\ 0 & 0 & 0 & \frac{4}{3}\frac{\eta}{\rho} + \frac{\mu}{\rho} \end{pmatrix}, \tag{5.66}$$

where κ, μ are thermal conductivity and bulk viscosity, respectively. Also $\rho = n_s m$ is the mass density.

The Explicit expressions for the equation of state and transport coefficients are following. First, the equation of the state is

$$p = p_0 \, (1 + \frac{2}{3}\pi n\sigma^3\chi), \tag{5.67}$$

where $p_0 = nk_BT$ and σ is the diameter of the hard sphere. The χ is the equilibrium pair correlation calculated at contact and is calculated from the Percus-Yevick approximation,

$$\chi = (1 - \frac{\pi n\sigma^3}{12} - \frac{(\pi n\sigma^3)^2}{72}) \, / \, (1 - \frac{\pi n\sigma^3}{6})^3. \tag{5.68}$$

The transport coefficients are

$$\eta = \frac{1}{\chi}(1 + \frac{4}{15}\pi n\sigma^3\chi)^2\eta_B + \frac{2}{5}\,\mu, \tag{5.69}$$

$$\mu = 1.002 \, (\frac{2}{3}\pi n\sigma^3)^2\chi \, \eta_B, \tag{5.70}$$

$$\kappa = \frac{1}{\chi}(1 + \frac{2}{5}\pi n\sigma^3\chi)^2\kappa_B + \mu C_v, \tag{5.71}$$

where $\mu C_v = 1.002/2.522\,(2/3\pi n\sigma^3)^2\chi\kappa_B$. In these expressions, η_B and κ_B are derived from the Boltzmann equation for hard spheres,

$$\eta_B = 1.016 \times \frac{5}{16}\sqrt{\frac{mk_BT}{\pi}}\sigma^{-2}, \tag{5.72}$$

$$\kappa_B = 1.088 \times \frac{15}{4}\frac{k_B}{m}\eta_B. \tag{5.73}$$

The dispersion relations are obtained from $\det(F_N - sI) = 0$ in order to find five hydrodynamic modes, $s_i(a,k)$, where $F_N = A_N - ikB_N + k^2D_N$. They are calculated for finite a and asymptotically small k explicitly to order k^2.

$$s_1 \to -(\frac{1}{2} + i\,\frac{\sqrt{3}}{2})c_2k^{2/3} - (\frac{1}{2} + i\,\frac{\sqrt{3}}{2})^2c_3k^{4/3} + (\frac{c_1}{3} + c_4)k^2, \tag{5.74}$$

$$s_2 = s_1^*, \tag{5.75}$$

$$s_3 \to c_1k^2, \tag{5.76}$$

$$s_4 \to c_2k^{2/3} - c_3k^{4/3} + c_4k^2, \tag{5.77}$$

$$s_5 \to \frac{\eta}{\rho}k^2, \tag{5.78}$$

$$\tag{5.79}$$

where

$$c_1 = \frac{k_BT}{2m}\frac{n}{p}[\frac{\eta}{p}\frac{\partial p}{\partial n} - 2\frac{\partial \eta}{\partial n}], \tag{5.80}$$

$$c_2 = \left(\frac{4k_BT}{3m}\frac{\eta a^2}{p}\right)^{1/3}, \tag{5.81}$$

$$c_3 = \frac{2k_BT}{9m}(1 + \eta^2\frac{a^2}{p^2} + \frac{n}{p}\frac{\partial p}{\partial n})/c_2, \tag{5.82}$$

$$c_4 = \frac{c_1}{3} + \frac{2\kappa}{3n_sk_B} + \frac{7\eta}{3\rho} + \frac{\mu}{\rho}. \tag{5.83}$$

These c_1, c_2, c_3 and c_4 are positive constants depending only on the density and temperature of the state. Since the first two complex conjugate pairs are negative for small k and finite a, s_4 and s_5 are unstable, while the other three modes are stable for small k and finite a. To compare the results with the ones from BGK-kinetic models (5.28)-(5.31), the same numerical value for shear rate ($a = 0.1$) can be used in these s_i's. They are

$$s_1 \xrightarrow{k\to 0} (-0.087 - 0.15\,i)\,k^{2/3} + (0.80 - 1.38\,i)\,k^{4/3} + 0.6\,k^2, \tag{5.84}$$

$$s_3 \xrightarrow{k\to 0} 0.20k^2, \tag{5.85}$$

$$s_4 \xrightarrow{k\to 0} 0.174\,k^{2/3} - 1.6\,k^{4/3} + 0.6\,k^2. \tag{5.86}$$

Notice that since these s_i are from $\det(F_N - sI)$, the negative means unstable. It proves that the instability is not a result from the BGK-kinetic models. Figure 5.1 shows the critical lines in the k-a plane separating stable (above) from unstable (below) dynamics at three different densities and also shows the results from the BGK-kinetic model. When the density is zero, the critical line is matched with the one from the BGK-kinetic model in the small shear rate region. It shows the same qualitative results for the two different models. Since the Navier-Stokes results are calculated for small gradients, the curves for the large shear rate region are outside the validity range. The "long wavelength instability" is clearly seen

in this figure. This instability gives a limited region to study the dynamics of the hydrodynamic modes. In next section, the stable dynamics are discussed and the two time correlation functions are calculated.

CHAPTER 6
EQUAL TIME CORRELATION FUNCTION

In the previous chapter, we studied the dynamics of the two time correlation functions. To complete the analysis, we need to know the initial conditions for those correlation functions. The initial condition is the equal time correlation function and represents time independent fluctuations within the reference state. While there have been some calculations of such fluctuations in stationary nonequilibrium states [2], most applications were limited to states near local equilibrium. Recently, accurate experimental results [4,29,38] have confirmed the predictions for these weakly nonequilibrium fluctuations. Here we calculate equal time correlation functions for a uniform shear flow state far from equilibrium using the kinetic model equation, Eq.(3.39), from Chapter 3. The same eigenvalue method which was developed in section 5.2 is used and the spatial long range (algebraic decay) correlation is shown to persist far from equilibrium. However, some limitations on the range occur due to the instability discussed in the last section.

In Chapter 3, we derived the kinetic model equation for the equal time correlation function, (3.39). The general solution to this equation for the stationary state, (3.64), can be written in Fourier representation as

$$\tilde{C}_s(\mathbf{k}_1, \mathbf{v}_1; \mathbf{k}_2, \mathbf{v}_2)$$

$$= \delta(\mathbf{k}_1 + \mathbf{k}_2)\delta(\mathbf{v}_1 - \mathbf{v}_2) f_s + \int_0^\infty dt\, e^{-(\tilde{\mathcal{L}}_1 + \tilde{\mathcal{L}}_2)t} \tilde{\gamma}(\mathbf{k}_1, \mathbf{v}_1; \mathbf{k}_2, \mathbf{v}_2) \tag{6.1}$$

$$= \delta(\mathbf{k}_1 + \mathbf{k}_2)\delta(\mathbf{v}_1 - \mathbf{v}_2) f_s + \tilde{G}_s(\mathbf{k}_1, \mathbf{v}_1; \mathbf{k}_2, \mathbf{v}_2). \tag{6.2}$$

The second term, $\tilde{G}_s$ is a stationary pair correlation function defined by Eq.(3.7). We notice that this pair correlation function has two of the operators, $\mathcal{L}$ used in the two time correlation function, here defined over functions of $\mathbf{v}_1$ and $\mathbf{v}_2$. Again, we limit attention to the long wavelength limit, for which the equal time matrix of the hydrodynamic correlations are appropriate (i.e. Eq(5.3) with $t = 0$)

$$\tilde{C}_{\alpha\beta}(\mathbf{k}_1, \mathbf{k}_2) = \int d\mathbf{v}_1 d\mathbf{v}_2\, \psi_\alpha(\mathbf{v}_1)\psi_\beta(\mathbf{v}_2)\tilde{C}_s(\mathbf{k}_1, \mathbf{v}_1; \mathbf{k}_2, \mathbf{v}_2), \tag{6.3}$$

$$= \delta(\mathbf{k}_1 + \mathbf{k}_2) \int d\mathbf{v}\, \psi_\alpha(\mathbf{v})\psi_\beta(\mathbf{v}) f_s(v) + \tilde{G}_{\alpha\beta}(\mathbf{k}_1, \mathbf{k}_2), \tag{6.4}$$

where

$$\tilde{G}_{\alpha\beta}(\mathbf{k}_1, \mathbf{k}_2) = \int d\mathbf{v}_2 d\mathbf{v}_2\, \psi_\alpha(\mathbf{v}_1)\psi_\beta(\mathbf{v}_2)\tilde{G}_s(\mathbf{k}_1, \mathbf{v}_1; \mathbf{k}_2, \mathbf{v}_2) \tag{6.5}$$

$$= \int_0^\infty dt \int d\mathbf{v}_1 d\mathbf{v}_2\, \psi_\alpha(\mathbf{v}_1)\psi_\beta(\mathbf{v}_2) e^{-(\tilde{\mathcal{L}}_1 + \tilde{\mathcal{L}}_2)t} \tilde{\gamma}(\mathbf{k}_1, \mathbf{v}_1; \mathbf{k}_2, \mathbf{v}_2 | f_s).$$

(6.6)

The first term of Eq.(6.4) is proportional to $\delta(\mathbf{k}_1 + \mathbf{k}_2)$ and represents short ranged spatial correlations as in the equilibrium case. The second term of Eq.(6.4), $\tilde{G}_{\alpha\beta}$, represents the hydrodynamic pair correlation function. At equilibrium, the hydrodynamic pair correlation function, $\tilde{G}_{\alpha\beta}$ is zero because $\tilde{\gamma}(f_e)$ in (6.6) vanishes by definition in (3.36).

However, at nonequilibrium, $\tilde{\gamma}$ is no longer zero and provides new nonequilibrium phenomena. At the states near equilibrium, the density fluctuations for uniform shear flow already have been calculated in the second example of section 3.4. They showed spatial algebraic decay of the fluctuations in (3.76). For states far from equilibrium (large shear rate), the hydrodynamic equal time correlation function also can be analyzed by using the eigenvalues and eigenvectors of $\tilde{\mathcal{L}}_1$ and $\tilde{\mathcal{L}}_2$. However, there is a limitation for the spatial range because of the instability discussed in the last chapter. Then the hydrodynamic eigenvalues should be calculated for limited region $k > k_c(a)$ (see Figure 5.1). Since the operators $\tilde{\mathcal{L}}_1$ and $\tilde{\mathcal{L}}_2$ are the same as those used for the two time correlation functions in the last chapter, the same hydrodynamic eigenvalues, s_i in (5.38)-(5.41) and the same eigenvectors, $\zeta^{(i)}$ in (5.42)-(5.45) can be used for the analysis of the pair correlation function. Then the hydrodynamic pair correlation (6.6) can be written in terms of these eigenvalues and eigenfunctions and the time integral performed to give

$$G_{\alpha\beta}(\mathbf{k}_1,\mathbf{k}_2) = \sum_{i,j} \frac{1}{(s_i(\mathbf{k}_1,x)+s_j(\mathbf{k}_2,x))} \zeta_\alpha^{(i)}(\mathbf{k}_1,x)\zeta_\beta^{(j)}(\mathbf{k}_2,x)H^{ij}(\mathbf{k}_1,\mathbf{k}_2,x), \quad (6.7)$$

where $x = kv_0/a$ is the variable used in the section 5.2. The matrix $H^{ij}(\mathbf{k}_1,\mathbf{k}_2,x)$ is defined by

$$\begin{aligned} &H^{ij}(\mathbf{k}_1,\mathbf{k}_2,x) \\ &\equiv \sum_{\gamma\sigma} \eta_\gamma^{(i)}(\mathbf{k}_1,x)\eta_\sigma^{(j)}(\mathbf{k}_2,x) \int d\mathbf{v}_1 d\mathbf{v}_2 \psi_\gamma(\mathbf{v}_1)\psi_\sigma(\mathbf{v}_2)\tilde{\gamma}(\mathbf{k}_1,\mathbf{v}_1;\mathbf{k}_2,\mathbf{v}_2) \end{aligned} \quad (6.8)$$

$$= \delta(\mathbf{k}_1 + \mathbf{k}_2) \sum_{\gamma\sigma} \eta_\gamma^{(i)}(\mathbf{k}_1, x)\eta_\sigma^{(j)}(\mathbf{k}_2, x)\nu \int d\mathbf{v}\psi_\gamma(\mathbf{v})\psi_\sigma(\mathbf{v})(f_s(\mathbf{v}) - f_{s\ell}(\mathbf{v})). \tag{6.9}$$

The second line of the equation is obtained using γ^{BGK} in (3.36) and the elements of H^{ij} are given in Appendix H.

Let us now specialize Eq.(6.7) to the density fluctuations for uniform shear flow, i.e. $\alpha = \beta = 1$,

$$\begin{aligned} G_{11}(\mathbf{k}_1, \mathbf{k}_2) = &\left(\frac{2}{5k^2} - \frac{2}{5}\frac{2}{k^2 + \frac{2}{5}a^2}\right) H^{11} + \frac{1}{k^2 + \frac{4}{5}a^2}\frac{2}{5}H^{22} \\ &- \frac{\sqrt{6}}{5}\frac{2(k^2 + a^2/5)}{\frac{5}{6}k^2 + (k^2 + \frac{a^2}{5})^2} 2\,\mathrm{Re}[H^{23}] + \frac{2}{k^2 - \frac{2}{5}a^2}\frac{3}{5}H^{33} \\ &+ \frac{2(k^2 - \frac{2}{5}a^2)}{\frac{5}{3}k^2 + (k^2 - \frac{2}{5}a^2)^2}\frac{3}{5}H^{34}, \end{aligned} \tag{6.10}$$

where k and a are used in units of ν/v_0 and ν for simplicity. This expression for the density fluctuation is restricted to $k > \sqrt{\frac{2}{5}}a$, and according to Figure 5.1 this k and a relation is valid for $a < 0.5$. When $a = 0$ (equilibrium case), G_{11} becomes zero which is the expected equilibrium result, and for finite a the correlation function shows long ranged spatial correlations.

CHAPTER 7
CONCLUSIONS

The objective in this thesis has been to study transport and fluctuations for states far from equilibrium for the special nonequilibrium states of uniform shear flow. Dynamical properties of states far from equilibrium are not well understood due to their complexity and technical difficulties with the formal theories of nonequilibrium statistical mechanics. However at low density, kinetic theory provides a controlled formulation of this problem. It consists of three kinetic equations: the Boltzmann equation, and related equations for the two time and equal time correlations. They describe all states from equilibrium to far from equilibrium. There are still difficulties for practical applications, except for cases at or close to equilibrium.

In this thesis, we constructed kinetic models corresponding to these kinetic equations in order to resolve practical difficulties for system far from equilibrium. The simple BGK model for the Boltzmann equation has been extended in a self-consistent way to apply to kinetic equations for fluctuations as well. All of the important structural relationships of the three kinetic equations are preserved by this model. If the solution to nonlinear BGK-Boltzmann equation is obtained, the linear equations for the two and equal time correlations can be solved. These kinetic model equations were applied to uniform shear flow to calculate transport properties and fluctuations for large shear rate. First, the BGK-Boltzmann

equation was solved for uniform shear flow and the normal solution was obtained near uniform shear flow by using a variant of the Chapman-Enskog approximation method. By "variant" we mean that in this expansion for uniform shear flow, the localized form of the stationary solution is used as a reference function instead of the local equilibrium distribution function. This normal solution consists of hydrodynamic variables and their spatial gradients,

$$f = f^{(0)}(n(\mathbf{r},t), T(\mathbf{r},t), \mathbf{u}(\mathbf{r},t)) + f^{(1)}(\nabla n, \nabla T, \nabla \delta \mathbf{u}). \tag{7.1}$$

This function then was used to calculate the irreversible momentum and heat fluxes in terms of the hydrodynamic gradients,

$$t^*_{ij} = -\eta \frac{\partial u_{s,i}}{\partial r_j} + \gamma^{ij}_{lk} \frac{\partial \delta u_l}{\partial r_k} \tag{7.2}$$

$$q^*_i = \xi^i_{T,j} \frac{\partial \delta T}{\partial r_j} + \xi^i_{n,j} \frac{\partial \delta n}{\partial r_j}, \tag{7.3}$$

where "*" denotes the irreversible part of these fluxes. The coefficients of these gradients are transport coefficients. Since these coefficients are calculated near the stationary state rather than at the local equilibrium state, there are many new coefficients (γ^{ij}_{lk}, $\xi^i_{T,j}$, $\xi^i_{n,j}$), which characterize the transport properties of the system far from equilibrium (i.e., for large shear rate). With these new expressions for the fluxes, a closed set of the generalized hydrodynamic equations was derived near uniform shear flow.

The equation of the two time correlation function for hydrodynamic fluctuations in uniform shear flow has the same dynamics as that for the linearized

hydrodynamic equations around the reference state. We studied the excitations (hydrodynamic modes) of the uniform shear flow by linearizing these hydrodynamic equations. It was verified that there exist hydrodynamic modes even far from equilibrium (i.e. modes that vanish as $k \to 0$). However, we also found that there is an instability for long wavelengths and any finite shear rate. This instability is compared with computer simulation results (by J. Montanero and A. Santos) and showed very good agreement between theory and simulation during the initial stages (see Figure 5.2). Because of the linear analysis in theory, the large time behavior could not be studied, but the simulation has been performed for longer times and shows continuing growth of the hydrodynamic variables. For the final stage of this instability, the simulation predicts a homogeneous state with a higher temperature. It is likely that the long wavelength instability has not been seen in previous molecular dynamics simulations due to the finite system sizes considered.

Finally the equal time correlations were investigated. The long ranged correlation in the density fluctuations was calculated for small and large shear rate. For states near equilibrium (small shear rate), the spatial algebraic decay of the fluctuations has been known for some time. Similar results were obtained here for large shear rate as well. However there is a spatial restriction this time because of the long wave length instability. The effect of this instability on both equal and two time correlations requires further study.

In this thesis, we applied the special nonequilibrium state of uniform shear flow to "model" kinetic equations in order to study transport and fluctuations.

These model equations also can be used for steady heat flow or combined heat and momentum fluxes, for which exact solutions to the BGK-Boltzmann equation are known [50, 51]. This will be deferred to future work. Also, it remains to understand the nature of the instability and its consequences. The directions of the perturbations can be generalized (e.g., $k_x \neq 0$) for analyzing the hydrodynamic modes. Then, we can obtain a more complete description of long range correlations (e.g., we can have a directionally dependent long range correlation). By using a BGK-Enskog equation, the system can be extended to higher densities where we can study the instability for conditions more suitable to molecular dynamics simulation. At high density, a large k hydrodynamic instability has been proposed [52, 53] and shown to occur at shear rates similar to those observed in the molecular dynamics simulations [9]. Further study is required to relate the mechanism in the large k hydrodynamic equations to that described in this thesis at small k.

APPENDIX A
DENSITY FLUCTUATIONS

In Chapter 2, density fluctuations are studied and long range spatial correlations are verified for small shear rate. In this appendix, a few steps to reach the results will be shown. The nonequilibrium part of density fluctuations (2.34) is written by using the analysis from Dufty [27] and Groome, Gubbins and Dufty [28] as

$$\begin{aligned}
&\lim_{t\to\infty}\langle\delta n(\mathbf{r})\delta n(\mathbf{r}')\widetilde{M}_{xy}(t)\rangle_e = \\
&-\frac{1}{(2\pi)^3}\int d\mathbf{k}\, i\frac{\partial}{\partial k_y}e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\int_0^\infty d\tau\,(p_x,\, nJ_s[\tilde{a}(\mathbf{k},\mathbf{v}),\tilde{a}(-\mathbf{k},\mathbf{v})]) \\
&-\frac{1}{(2\pi)^3}\int d\mathbf{k}\, e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\int_0^\infty d\tau\,\left(I^{-1}\frac{v_x v_y}{m},\, J_s[\tilde{a}(\mathbf{k},\mathbf{v})\tilde{a}(-\mathbf{k},\mathbf{v})]\right),
\end{aligned} \tag{A.1}$$

where (X, Y) is defined by

$$(X, Y) = \int d\mathbf{p}\, f_0\, X\, Y, \tag{A.2}$$

and

$$\tilde{a}(\mathbf{k},\mathbf{v}) \equiv e^{-t(nI-i\mathbf{k}\cdot\mathbf{v})}1. \tag{A.3}$$

The $\tilde{a}$ function depends on the inhomogeneous linearized Boltzmann operator $nI - i\mathbf{k}\cdot\mathbf{v}$ and can be represented in terms of its proper eigenvalues and

eigenvectors. To solve equation (A.1), first write the function $\tilde{a}$ in terms of combination of eigenvectors of $nI - i\mathbf{k}\cdot\mathbf{v}$

$$(nI - i\mathbf{k}\cdot\mathbf{v})g_\alpha = s_\alpha g_\alpha, \tag{A.4}$$

where s_α, g_α are eigenvalues, eigenvectors respectively. This equation is solved by perturbation theory for small wavevectors. The dominant contribution for long range correlations arises from the hydrodynamic spectrum (eigenvalues that vanishes as $k \to 0$). The hydrodynamic eigenvalues and eigenvectors can be found in the literature [54], so only the results are given:

$$\begin{aligned} g_{1,2} = &\sqrt{\frac{2}{15}}\left\{\frac{\epsilon}{k_BT} + \frac{ik}{p}[\hat{k}\cdot\mathcal{S} + \frac{1}{2}\eta(1-\frac{1}{2}\theta)\hat{k}\cdot\mathbf{v}]\right\} \\ &\mp\sqrt{\frac{m}{2k_BT}}\left\{\mathbf{k}\cdot\mathbf{v} + \frac{ik}{m}[\hat{k}\mathcal{T}\hat{k} - \frac{2}{15}\eta(1-\frac{7}{2}\theta)\frac{\epsilon}{k_BT} - \theta\eta]\right\}, \end{aligned} \tag{A.5}$$

$$g_3 = \sqrt{\frac{m}{k_BT}}\left(\hat{e}_1\cdot\mathbf{v} + \frac{i\,k}{p}\hat{k}\mathcal{T}\hat{e}_1\right), \tag{A.6}$$

$$g_4 = \sqrt{\frac{m}{k_BT}}\left(\hat{e}_2\cdot\mathbf{v} + \frac{i\,k}{p}\hat{k}\mathcal{T}\hat{e}_2\right), \tag{A.7}$$

$$g_5 = \sqrt{\frac{2}{5}}\left[\frac{\epsilon}{k_BT} - \frac{5}{2} + \frac{i\,k}{p}(\hat{k}\cdot\mathcal{S} - \theta\eta\hat{k}\cdot\mathbf{v})\right], \tag{A.8}$$

with eigenvalues

$$s_{1,2} = \pm i\,k\,c + \Gamma k^2,\ s_3 = s_4 = \eta/(nm)k^2,\ s_5 = D_T k^2. \tag{A.9}$$

Here the wavevector is $\mathbf{k} = k\hat{k}$ and the orthogonal directions to $\mathbf{k}$ are given by

the unit vectors $\{\hat{e}_1, \hat{e}_2\}$. Also $\epsilon = \frac{1}{2}mv^2$ and $\mathcal{S}$, $\mathcal{T}$ are solutions to

$$I\mathcal{S}_i = S_i, \; I\mathcal{T}_{ij} = T_{ij}, \tag{A.10}$$

where S_i and T_{ij} are

$$S_i = \left(\frac{1}{2}mv^2 - \frac{5}{2}k_BT\right) v_i, \;\; T_{ij} = m\left(v_iv_j - \frac{1}{3}\delta_{ij}v^2\right). \tag{A.11}$$

The solutions, $\mathcal{S}$ and $\mathcal{T}$ exist due to the orthogonality of S_i and T_{ij} to the summational invariants. In Eqs.(A.5) and (A.8), $\theta = 2\kappa m/5k_B\eta$ is a dimensionless parameter and κ, η are the thermal conductivity and shear viscosity, respectively. In the eigenvalues, $c = \sqrt{5k_BT/3m}$ is the sound velocity, and Γ and D_T are the sound damping constant and thermal diffusivity. The normalization of eigenvectors is chosen such that $(h_\alpha, \, g_\beta) = \delta_{\alpha\beta}$, where $h_\alpha (= g_\alpha^*)$ are complex conjugates of g_α. Now the function $\tilde{a}$ is expressed in terms of these hydrodynamic eigenvectors,

$$\tilde{a}(\mathbf{k}, \mathbf{v}) \to \sum_{\alpha=1}^{5} c_\alpha e^{-s_\alpha(k)\tau} g_\alpha. \tag{A.12}$$

Consequently $J_s[\tilde{a}(k), \tilde{a}(-k)]$ can be written

$$\begin{aligned}
&J_s[\tilde{a}(\mathbf{k}, \mathbf{v}), \tilde{a}(-\mathbf{k}, \mathbf{v})] = \\
&c_1c_2e^{-2\Gamma k^2\tau}(J_s[g_1, h_1] + J_s[g_2, h_2]) + c_5^2e^{-2D_Tk^2\tau}J_s[g_5, h_5] \\
&+c_1^2e^{-2\tau(ikc+\Gamma k^2)}J_s[g_1, h_2] + c_2^2e^{2\tau(ikc-\Gamma k^2)}J_s[g_2, h_1] \\
&+c_1c_5e^{-\tau(ikc+\Gamma k^2+D_Tk^2)}(J_s[g_1, h_5] + J_s[g_5, h_2])
\end{aligned}$$

$$+c_2c_5\mathrm{e}^{-\tau(-ik\,c+\Gamma k^2+D_T k^2)}(J_s[g_2,h_5]+J_s[g_5,h_1]), \tag{A.13}$$

where

$$c_{1,2}=\frac{3}{2}\sqrt{\frac{2}{15}}\mp\frac{ik}{p}\sqrt{\frac{m}{2k_BT}}\left\{\frac{1}{5}\eta(1-\frac{7}{2}\theta)+\theta\eta\right\}, \tag{A.14}$$

$$c_5=-\sqrt{\frac{2}{5}}. \tag{A.15}$$

Use of this expression for $J_s[\tilde{a}(k),\tilde{a}(-k)]$ in Eq.(A.1) shows that the first term on the right side of Eq.(A.1) vanishes because the term $(p_x, nJ_s[\tilde{a}(\mathbf{k},\mathbf{v}),\ \tilde{a}(-\mathbf{k},\mathbf{v})])$ becomes zero due to the momentum conservation. Then Eq.(A.1) is

$$\begin{aligned}&\lim_{t\to\infty}\langle\delta n(\mathbf{r})\delta n(\mathbf{r}')\widetilde{M}_{xy}(t)\rangle_e\\&=-\frac{1}{(2\pi)^3}\int d\mathbf{k}e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\int_0^\infty d\tau\left(I^{-1}\frac{v_xv_y}{m},\ J_s[\tilde{a}(k),\tilde{a}(-k)]\right)\end{aligned} \tag{A.16}$$

$$=-\frac{1}{(2\pi)^3}\int d\mathbf{k}e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\int_0^\infty d\tau\frac{1}{m^2}(\mathcal{T}_{xy},\ nJ_s[\tilde{a}(k),\tilde{a}(-k)]). \tag{A.17}$$

Substitution of Eq.(A.13) in the integral of the right side of (A.17) leads to

$$\begin{aligned}&(\mathcal{T}_{xy},nJ_s[\tilde{a}(k),\tilde{a}(-k)])=-2c_1c_2\beta n(T_{xy},T_{xy})k_xk_y/k^2\,e^{-2\Gamma k^2\tau}\\&+\beta n(T_{xy},T_{xy})k_xk_y/k^2(c_1^2\mathrm{e}^{-2\tau ikc}+c_2^2\mathrm{e}^{2\tau ikc})\mathrm{e}^{-2\tau\Gamma k^2}\\&-2i\,k\frac{\beta^{3/2}}{\sqrt{15m}}[2(\mathcal{T}_{xy},(\epsilon+3/2T)T_{xy})k_xk_y/k^2-(T_{xy},\epsilon\mathcal{T}_{jj})\\&+m(\mathcal{T}_{xy},(v_xS_y+v_yS_x))k_xk_y/k^2-m(T_{xy},(v_y\mathcal{S}_x+v_x\mathcal{S}_y))k_xk_y/k^2\end{aligned}$$

$$
\begin{aligned}
&-2\eta/2(1-\theta/2)(T_{xy},T_{xy})k_xk_y/k^2](c_1^2e^{-2\tau\imath kc}-c_2^2e^{2\tau\imath kc})e^{-2\tau\Gamma k^2}\\
&+2i\,k\frac{\beta^{3/2}}{5m}[m(\mathcal{T}_{xy},(v_xS_y+v_yS_x))k_xk_y/k^2\\
&-m(T_{xy},(v_x\mathcal{S}_y+v_y\mathcal{S}_x))k_xk_y/k^2-2\theta\eta(T_{xy},T_{xy})k_xk_y/k^2\\
&-2(\mathcal{T}_{xy},(\epsilon+3/2\,T)T_{xy})k_xk_y/k^2+(T_{xy},\epsilon\mathcal{T}_{jj})+5(\mathcal{T}_{xy},T_{xy})k_xk_y/k^2]\\
&\times(c_1c_5e^{-\tau\imath kc}-c_2c_5e^{\tau\imath kc})e^{-\tau(\Gamma+D_T)k^2}. \qquad \text{(A.18)}
\end{aligned}
$$

After performing time integral and inverting the Fourier transformation, the leading term of the nonequilibrium part of the density fluctuation for large $|r-r'|$ is found to be

$$
\lim_{t\to\infty}\langle\delta n(\mathbf{r}\delta n(\mathbf{r}')\widetilde{M}_{xy}(t)\rangle_e=\frac{3}{80}\frac{nk_BT}{\pi\Gamma}\frac{(x-x')(y-y')}{(r-r')^3}+O[r^{-2}]. \qquad \text{(A.19)}
$$

Therefore the density fluctuation for uniform shear flow is

$$
\langle\delta n(\mathbf{r}\delta n(\mathbf{r}')\rangle_{ne}\sim\langle\delta n(\mathbf{r})\delta n(\mathbf{r}')\rangle_e-a\frac{3}{80}\frac{n}{\pi\Gamma}\frac{(x-x')(y-x')}{(r-r')^3}. \qquad \text{(A.20)}
$$

APPENDIX B
DERIVATION OF KINETIC EQUATIONS

In this appendix, the three kinetic equations (3.11)-(3.13) are derived from an approximation of BBGKY hierarchy by an expansion in powers of a low density parameter. The expansion parameter is obtained by scaling space and time with characteristic scales. Since we are interested in the phenomena that change appreciably over scales such as mean free path ($\ell_0 \equiv 1/n\sigma^2$) and mean free time ($t_0 \equiv \ell_0/v_0$), they are used as characteristic units to form a dimensionless hierarchy. Here, n is the density, σ is the force range, $v_0 = (2k_BT/m)^{1/2}$ is the average thermal velocity, and k_B, T and m are Boltzmann constant, temperature and the particle mass. With these scalings, the reduced distribution function $f^{(s)}$ is scaled with n^s/v_0^{3s}.

To simplify the analysis, we consider a gas of hard spheres, but the same results can be obtained for general short ranged forces by more elaborate methods [19,30]. Since the hard sphere interaction is singular, the forces are replaced by binary scattering operators [31]. The resulting dimensionless BBGKY hierarchy has the form

$$\left(\frac{\partial}{\partial t} + \sum_{i=1}^{s} \mathbf{v}_i \cdot \nabla_i - \alpha^2 \sum_{i<j}^{s} T(i,j)\right) f^{(s)}(y_1, \cdots, y_s, t)$$
$$= \sum_{i=1}^{s} \int dy_{s+1}\, T(i, s+1) f^{(s+1)}(y_1, \cdots, y_{s+1}, t). \tag{B.1}$$

$T(i,j)$ is an operator describing the scattering of the pair of particles $\{i,j\}$,

$$T(i,j) = \int d\hat{\mathbf{r}}\,\Theta(\mathbf{r}\cdot\mathbf{g}_{ij})\hat{\mathbf{r}}\cdot\mathbf{g}_{ij}\left(\delta(\mathbf{r}_{ij}-\alpha\hat{\mathbf{r}})b_{ij}-\delta(\mathbf{r}_{ij}+\alpha\hat{\mathbf{r}})\right), \tag{B.2}$$

where $d\hat{\mathbf{r}}$ denotes a two dimensional solid angle integration over the sphere for particle at contact. Also $\mathbf{g}_{ij}\equiv\mathbf{v}_i-\mathbf{v}_j$ is the relative velocity, $\hat{\mathbf{r}}$ is a unit vector along the $\mathbf{r}_{ij}$, and b_{ij} is the scattering operator defined for any function $X(\mathbf{v}_i,\mathbf{v}_j)$ by

$$b_{ij}X(\mathbf{v}_i,\mathbf{v}_j)\equiv X(\mathbf{v}_i',\mathbf{v}_j'). \tag{B.3}$$

The scattered velocities are $\mathbf{v}_i'\equiv\mathbf{v}_i-(\mathbf{g}_{ij}\cdot\hat{\mathbf{r}})\hat{\mathbf{r}}$ and $\mathbf{v}_j'\equiv\mathbf{v}_j+(\mathbf{g}_{ij}\cdot\hat{\mathbf{r}})\hat{\mathbf{r}}$.

Equations (B.1) and (B.2) depend on the single dimensionless parameter $\alpha\equiv\sigma/\ell_0=n\sigma^3$, the ratio of the force range to the mean free path. This parameter is small at low density and can be used as an expansion parameter for the solutions to Eq.(B.1). The s-particle reduced distribution is expanded in powers of α,

$$f^{(s)}(y_1,\cdots,y_s,t)=\sum_{n=0}^{\infty}\alpha^{2n}f_n^{(s)}(y_1,\cdots,y_s,t). \tag{B.4}$$

Substituting Eq.(B.4) into the Eq. (B.1) and equating coefficients of α^{2n} gives the kinetic equations determining the coefficients $f_n^{(s)}$. The dependence of α in the operator $T(i,j)$ is neglected because the distances of interest are large compared to the force range, and the position difference between colliding partners can be neglected. Consequently $T(i,j)$ simplifies to

$$T(i,j)=\delta(\mathbf{r}_{ij})\int d\hat{\mathbf{r}}\,\Theta(\mathbf{r}\cdot\mathbf{g}_{ij})\hat{\mathbf{r}}\cdot\mathbf{g}_{ij}(b_{ij}-1). \tag{B.5}$$

To zeroth order in α the solutions are found to be

$$f_0^{(s)}(y_1, \cdots, y_s, t) = \prod_{i=1}^{s} f_0^{(1)}(y_i, t), \tag{B.6}$$

where $f_0^{(1)}$ is the solution to the kinetic equation

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_1 \cdot \nabla_1\right) f_0^{(1)}(y_1, t) = \int dy_2 \, T(1,2) f_0^{(1)}(y_1, t) f_0^{(1)}(y_2, t). \tag{B.7}$$

The binary collision operator, the right side of the Eq.(B.7), is recognized as the nonlinear Boltzmann operator for hard spheres, so $f_0^{(1)}$ is indeed the solution to the Boltzmann equation.

The solution to order α^2 is

$$f_1^{(2)}(y_1, y_2, t) = f_0^{(1)}(y_1, t) f_1^{(1)}(y_2, t) + f_0^{(1)}(y_2, t) f_1^{(1)}(y_1, t) + G_1(y_1, y_2, t). \tag{B.8}$$

The s-particle distribution function $f_1^{(s)}$ can be determined in terms of single particle function $f_0^{(1)}, f_1^{(1)}$ and pair function G_1, but will not be considered here. The functions $f_1^{(1)}$ and G_1 are the solutions to

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_1 \cdot \nabla_1 - \Lambda_1\right) f_1^{(1)}(y_1, t) = \int dy_2 \, T(1,2) G_1(y_1, y_2, t), \tag{B.9}$$

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_1 \cdot \nabla_1 - \Lambda_1 + \mathbf{v}_2 \cdot \nabla_2 - \Lambda_2\right) G_1(y_1, y_2, t) = T(1,2) f_0^{(1)}(y_1, t) f_0^{(1)}(y_2, t). \tag{B.10}$$

Here Λ_1 is the operator defined over functions of y_1 by

$$\Lambda_1 X(y_1) \equiv \int dy_2 T(1,2)(f_0^{(1)}(y_1,t)X(y_2) + X(y_1)f_0^{(1)}(y_2,t)). \tag{B.11}$$

This α expansion gives the exact solution to the entire hierarchy up to order α^2. The reduced distribution functions are determined as a sum of products of single particle functions $f_0^{(1)}(y_1,t)$, $f_1^{(1)}(y_1,t)$ and the pair function $G_1(y_1,y_2,t)$. From the definition of single time pair correlation $G(y_1,y_2,t)$ in (3.7) and the zeroth order solution (B.6), it is easily shown that the pair function $G_1(y_1,y_2,t)$ is a leading contribution to the density expansion of $G(y_1,y_2,t)$. Therefore in the low density limit, $G(y_1,y_2,t)$ is the solution to Eq.(B.10).

The analysis of correlations at two times can be accomplished in a similar way. Define the two time distribution function

$$h^{(s+1)}(y_1,\cdots,y_s,t;y',t') \equiv \langle \hat{f}^{(s)}(y_1,\cdots,y_s,t)\hat{f}^{(1)}(y',t')). \tag{B.12}$$

The two time correlation function in (3.6) is related to $h^{(2)}$ by

$$C(y,t:y',t') = h^{(2)}(y,t;y',t') - f^{(1)}(y,t)f^{(1)}(y',t'). \tag{B.13}$$

The two time distribution function $h^{(s)}$ obeys the same BBGKY hierarchy (B.1) for $t > t'$. When a power expansion in α is applied, the solution up to order α^2 is

$$h_0^{(s+1)}(y_1,\cdots,y_s,t;y',t') = f_0^{(1)}(y',t')f_0^{(s)}(y_1,\cdots,y_s,t), \tag{B.14}$$

$$h_1^{(2)}(y_1,t;y',t') = f_0^{(1)}(y_1,t)f_1^{(1)}(y',t') + f_1^{(1)}(y_1,t)f_0^{(1)}(y',t'), \tag{B.15}$$

and for $s \geq 2$

$$\begin{aligned} h_1^{(s+1)}(y_1,\cdots,y_s,t;y',t') &= f_0^{(s)}(y_1,\cdots,y_s,t)f_1^{(1)}(y',t') \\ &+ f_1^{(s)}(y_1,\cdots,y_s,t)f_0^{(1)}(y',t') + \sum_{i=1}^{s}\prod_{j\neq i}^{s} f_0^{(1)}(y_j,t)C_1(y_i,t;y',t'), \end{aligned} \tag{B.16}$$

where C_1 obeys the equation

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla - \Lambda\right) C_1(y,t;y',t') = 0, \tag{B.17}$$

for $t \geq t'$. Substitution of (B.16) into (B.13) shows that $C_1(y,t;y',t')$ is the first nonvanishing contribution to $C(y,t;y',t')$, so that $C(y,t;y',t')$ satisfies Eq.(B.17) at the low density limit. This completes the derivation of all low density kinetic equations for transport and pair correlations at one and two times.

APPENDIX C
DERIVATION OF KINETIC MODEL

In this appendix, the operator Λ^{BGK} (3.31) is derived in detail. The model for the linear operator Λ is obtained from the functional relation to the Boltzmann collision operator,

$$\Lambda^{\mathrm{BGK}} h(y) \equiv \int dy_1 \left(\frac{\delta}{\delta f(y_1,t)} J^{\mathrm{BGK}}(y|f(t)) \right) h(y_1)$$

$$= -\nu \left(h(y) - \int dy_1 \, h(y_1) \frac{\delta}{\delta f(y_1,t)} f_\ell(y,t) \right). \tag{C.1}$$

Here $J^{\mathrm{BGK}} = -\nu(f - f_\ell)$ is used. The functional dependence of f_ℓ on f occurs only through the the functions z_α. These functions are defined by

$$\int d\mathbf{v} \psi_\alpha(\mathbf{v}) f(y,t) = \int d\mathbf{v} \psi_\alpha(\mathbf{v}) f_\ell(y,t), \tag{C.2}$$

where $\psi_\alpha = \{1, \mathbf{v}, v^2\}$. This definition assumes that the BGK model retains the exact conservation laws. Therefore the functional derivative form of f_ℓ on f is written as

$$\frac{\delta}{\delta f(y_1,t)} f_\ell(y,t) = f_\ell(y,t) \psi_\alpha(\mathbf{v}) \frac{\delta}{\delta f(y_1,t)} z_\alpha(\mathbf{r},t). \tag{C.3}$$

Take the functional derivative of each side of (C.2) to get

$$\begin{aligned}\delta(\mathbf{r}-\mathbf{r}_1)\psi_\alpha \mathbf{v}_1 &= \int d\mathbf{v}\psi_\alpha(\mathbf{v})\frac{\delta}{\delta f(y_1,t)}f_\ell(y,t) \\ &= \int d\mathbf{v}\psi_\alpha(\mathbf{v})f_\ell(y,t)\psi_\beta(\mathbf{v})\frac{\delta}{\delta f(y_1,t)}z_\beta(\mathbf{r},t) \\ &= g_{\alpha\beta}(\mathbf{r},t)\frac{\delta}{\delta f(y_1,t)}z_\beta(\mathbf{r},t), \end{aligned} \tag{C.4}$$

where $g_{\alpha\beta}$ is defined by

$$g_{\alpha\beta}(\mathbf{r},t) \equiv \int d\mathbf{v}\, f_\ell(y,t)\psi_\alpha(\mathbf{v})\psi_\beta(\mathbf{v}). \tag{C.5}$$

Inversion of (C.4) for the functional derivatives gives

$$\frac{\delta}{\delta f(y_1,t)}z_\alpha(\mathbf{r},t) = \delta(\mathbf{r}-\mathbf{r}_1)\, g^{-1}_{\alpha\beta}(\mathbf{r},t)\psi_\beta(\mathbf{v}_1). \tag{C.6}$$

Put this form into (C.3) to get

$$\frac{\delta}{\delta f(y_1,t)}f_\ell(y,t) = f_\ell(y,t)\delta(\mathbf{r}-\mathbf{r}_1)\psi_\alpha(\mathbf{v})g^{-1}_{\alpha\beta}(\mathbf{r},t)\psi_\beta(\mathbf{v}_1). \tag{C.7}$$

This result is used with Eq.(C.1) to give the BGK model for operator Λ

$$\Lambda^{\mathrm{BGK}}h(y) = -\nu(1-P)h(y), \tag{C.8}$$

where $P(t)$ is defined in Eq.(3.32), and is a projection operator along the summational invariants, ψ_α.

APPENDIX D
EQUILIBRIUM EXCITATION

The dynamics of correlations at an equilibrium state is determined from the matrix $B_{\alpha\beta} = \delta_{\alpha\beta} - I_{\alpha\beta}$, Eq. (3.60), which determines both the hydrodynamic and kinetic poles. The matrix $I_{\alpha\beta}$ is obtained from the Fourier-Laplace transform of (3.51), specialized to the equilibrium state

$$\tilde{I}_{\alpha\beta}(k,z) = \nu\, g^{-1}_{\alpha\gamma} \int d\mathbf{v} f_e(\mathbf{v}) R(\mathbf{k}, z|\mathbf{v}) \psi_\gamma(\mathbf{v}) \psi_\beta(\mathbf{v}), \tag{D.1}$$

where $R(\mathbf{k}, z|\mathbf{v})$ is given by (3.59). Further analysis is simplified by choosing the collisional invariants $\psi_\alpha(\mathbf{v})$ to be an orthonormal set, $\phi_\alpha(\mathbf{v})$, constructed from linear combinations of those in (3.22),

$$\phi_\alpha(\mathbf{v}) = \left\{ 1, \sqrt{\frac{2}{3}} \left(\frac{mv^2}{2k_BT} - \frac{3}{2} \right), \sqrt{\frac{m}{k_BT}}\, v_1, \sqrt{\frac{m}{k_BT}}\, v_2, \sqrt{\frac{m}{k_BT}}\, v_3 \right\}, \tag{D.2}$$

where $v_1 \equiv \hat{\mathbf{k}} \cdot \mathbf{v}$ is the component of $\mathbf{v}$ along $\mathbf{k}$, and v_2 and v_3 are the orthogonal transverse components. With this choice, $g_{\alpha\beta} = n\, \delta_{\alpha\beta}$ and (D.1) reduces to

$$\tilde{I}_{\alpha\beta}(k,z) = \frac{i\nu}{kv_0} A_{\alpha\beta}(x). \tag{D.3}$$

Here the dimensionless variable $x \equiv (z+\nu)/ikv_0$ is used, and $v_0 = (2k_BT/m)^{1/2}$ is the thermal velocity. $A_{\alpha\beta}$ is a symmetric matrix and its elements are given in

terms of the complex probability integral,

$$Z(x) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dv \, \frac{\exp -v^2}{v - x}, \tag{D.4}$$

by

$$(A_{\alpha\beta}) = \begin{pmatrix} Z & (\frac{2}{3})^{1/2}[x + (x^2 - \frac{1}{2})Z] & \sqrt{2}(1 + xZ) & 0 & 0 \\ A_{12} & \frac{2}{3}[Z + (\frac{3}{2})^{1/2}(x^2 - \frac{1}{2})A_{12}] & \sqrt{2}xA_{12} & 0 & 0 \\ A_{13} & A_{23} & \sqrt{2}xA_{13} & 0 & 0 \\ 0 & 0 & 0 & Z & 0 \\ 0 & 0 & 0 & 0 & Z \end{pmatrix}. \tag{D.5}$$

Since $\tilde{I}_{\alpha\beta}$ is analytic for $Re(z) \neq -\nu$, the singularities of $B^{-1}_{\alpha\beta}(k, z)$ leading to hydrodynamic modes are associated with values of z for which

$$\det (B_{\alpha\beta}) = \det (\delta_{\alpha\beta} - \tilde{I}_{\alpha\beta}) = 0, \tag{D.6}$$

and vanish as $k \to 0$. This equation is solved numerically to look for five hydrodynamic dispersion relations, $z = z(k)$, such that $z(k = 0) = 0$. In fact due to the structure of the matrix $A_{\alpha\beta}$, Eq.(D.6) factorizes into two independent equations.

$$\det(B_{\alpha\beta}) = \frac{1}{6}(1 - \frac{i\nu Z}{kv_0})^2(M(k, z) + iN(k, z)) = 0. \tag{D.7}$$

The first equation gives a twofold real degenerate solution, $z_s(k)$, and there is a maximum value of k, $k^*_s = \sqrt{\pi}\nu/v_0$, where the first equation no longer has a solution. When $k = k^*_s$, the value of $z(k^*) = -\nu$. This branch represents

the shear modes defined for $k < k_s^*$. To lowest order in k, one gets the familiar Navier-Stokes expression $z_s = -\eta k^2$, where $\eta = p/\nu$ is the kinematic viscosity.

The other equation, $M + iN = 0$, leads to two solutions which are complex conjugates and to another real solution. These are the two sounds mode, $z_\pm$, and the heat mode, z_H, respectively. To Navier-Stokes order, $z_\pm = \pm ick - \Gamma k^2$ and $z_H = -D_T k^2$, where c is the sound velocity, Γ is the sound damping constant, and D_T is the thermal diffusivity. For the BGK model, $\eta = \Gamma = D_T$, in agreement with what is observed in Fig.(3.1). The sound modes and the heat mode also present limiting values of k. From our numerical analysis we have found $k_\pm^* \simeq 1.85\nu/v_0$ and $k_H^* \simeq 1.91\nu/v_0$, corresponding to $z_\pm = z_H = -\nu$.

APPENDIX E
FIRST ORDER APPROXIMATION

In this appendix, the first order equation, (4.35) is solved. Eq.(4.35) is

$$\left(D_t^{(1)} + \mathbf{v}' \cdot \nabla\right) f^{(0)} = -\left(\frac{\partial^{(0)}}{\partial t} - L(v', a) + \lambda \delta u_i \frac{\partial}{\partial v_i'} + \nu\right) f^{(1)}, \tag{E.1}$$

where $D_t^{(1)} \equiv \frac{\partial^{(1)}}{\partial t} + a_{ij} r_j \frac{\partial}{\partial r_i}$. The terms on the left side of Eq.(E.1) can be written as

$$(D_t^{(1)} + \mathbf{v}' \cdot \nabla) f^{(0)} = \sum_{\alpha=1}^{5} \frac{\partial f^{(0)}}{\partial y_\alpha} (D_t^{(1)} + \mathbf{v}' \cdot \nabla) y_\alpha, \tag{E.2}$$

where y_α denotes $\{n(\mathbf{r}, t), T(\mathbf{r}, t), \delta\mathbf{u}(\mathbf{r}, t)\}$. Those time derivatives can be replaced by first order spatial gradients of hydrodynamic variables by using the corresponding hydrodynamic equations obtained from Eqs.(4.8), (4.9) and (4.10) to first order in the gradients

$$D_t^{(1)} n + \nabla \cdot n\delta\mathbf{u} = 0, \tag{E.3}$$

$$\frac{3}{2} n k_B (D_t^{(1)} + \delta\mathbf{u} \cdot \nabla) T + a_{ij} t_{ij}^{(1)} + t_{ij}^{(0)} \frac{\partial \delta u_i}{\partial r_j} + \nabla \cdot \mathbf{q}^{(0)} = 0, \tag{E.4}$$

$$D_t^{(1)} \delta u_l + \delta\mathbf{u} \cdot \nabla \delta u_l + \rho^{-1} \frac{\partial t_{il}^{(0)}}{\partial r_i} = 0. \tag{E.5}$$

Use of these equations into Eq.(E.2) gives

$$(D_t^{(1)} + \mathbf{v}' \cdot \nabla) f^{(0)} = Y_{n,i} \frac{\partial n}{\partial r_i} + Y_{T,i} \frac{\partial T}{\partial r_i} + Y_{u_n,i} \frac{\partial \delta u_n}{\partial r_i}. \tag{E.6}$$

The coefficients, $Y_{\alpha,i}$, are given by

$$Y_{n,i} = \frac{\partial f^{(0)}}{\partial n}(v_i' - \delta u_i) - \rho^{-1} \frac{\partial f^{(0)}}{\partial \delta u_l} \frac{\partial t_{il}^{(0)}}{\partial n}, \tag{E.7}$$

$$Y_{T,i} = \frac{\partial f^{(0)}}{\partial T}(v_i' - \delta u_i) - \rho^{-1} \frac{\partial f^{(0)}}{\partial \delta u_l} \frac{\partial t_{il}^{(0)}}{\partial T}, \tag{E.8}$$

$$Y_{u_k,i} = -n \frac{\partial f^{(0)}}{\partial n} \delta_{ki} - \frac{2}{3nk_B} \frac{\partial f^{(0)}}{\partial T} \left(t_{ki}^{(0)} + a_{lm} \frac{\partial t_{lm}^{(1)}}{\partial \left(\frac{\partial \delta u_k}{\partial r_i} \right)} \right) + \frac{\partial f^{(0)}}{\partial u_k}(v_i' - \delta u_i), \tag{E.9}$$

where i, l, k denote x, y, z. The derivative of $f^{(0)}$ is simply obtained by

$$\frac{\partial f^{(0)}}{\partial n} = \frac{f^{(0)}}{n} + \left(\frac{\partial \nu}{\partial n} \right) \frac{1}{\nu} [f^{(0)} - h_n], \tag{E.10}$$

$$\frac{\partial f^{(0)}}{\partial T} = -\frac{3}{2T} f^{(0)} + \frac{m}{2k_B T^2} \nu h_T, \tag{E.11}$$

$$\frac{\partial f^{(0)}}{\partial \delta u_l} = \frac{m}{k_B T} \nu h_{u_l}. \tag{E.12}$$

Here the functions h_α are defined with time integration,

$$h_n = \int_0^\infty d\tau \, \tau e^{-\nu\tau + 3\lambda\tau} f_\ell (e^{\lambda\tau} \Lambda_{ij}(-\tau)(v_j' - \delta u_j)), \tag{E.13}$$

$$h_T = \int_0^\infty d\tau \, e^{-\nu\tau + 3\lambda\tau} e^{2\lambda\tau} [\Lambda_{ij}(-\tau)(v_j' - \delta u_j)]^2 f_\ell (e^{\lambda\tau} \Lambda_{ij}(-\tau)(v_j' - \delta u_j)), \tag{E.14}$$

$$h_{u_k} = \int_0^\infty d\tau\, \mathrm{e}^{-\nu\tau+3\lambda\tau}\mathrm{e}^{2\lambda\tau} g_k(\mathbf{v}',\tau) f_\ell(\mathrm{e}^{\lambda\tau}\Lambda_{ij}(-\tau)(v_j' - \delta u_j)), \tag{E.15}$$

where $g_k(\mathbf{v}',t)$ in the h_{u_k} are

$$\begin{aligned} g_x &= (v_x' - \delta u_x) + at(v_y' - \delta u_y), \\ g_y &= at(v_x' - \delta u_x) + (1 + a^2t^2)(v_y' - \delta u_y), \\ g_z &= v_z' - \delta u_z. \end{aligned} \tag{E.16}$$

Now the left side of Eq.(E.1) can be written in terms of known coefficients, $Y_{\alpha,i}$ and hydrodynamic gradients. The right side of Eq.(E.1) can be written in terms of hydrodynamic gradients and unknown coefficients, $X_{\alpha,i}$, which was defined in (4.46). By equating the coefficients of the hydrodynamic gradients in both side of equation finally gives the equations for $X_{\alpha,k}$.

$$\left(\frac{\partial^{(0)}}{\partial t} - L(v',a) + \lambda\, \delta u_i \frac{\partial}{\partial v_i'} + \nu\right) X_{\alpha,k} - aX_{u_x,k}\delta_{\alpha,u_y} = -Y_{\alpha,k}, \tag{E.17}$$

where $\alpha = n, T, u_x, u_y, u_z$. The last term on the left side of Eq.(E.17) exists due to the time dependence of the homogeneous solution of $\delta u_x(t)$ in Eq.(5.17). This equation has a form similar to Eq.(4.34) and the general solution can be written as

$$\begin{aligned} X_{\alpha,k} = \int_0^\infty d\tau\, \mathrm{e}^{-\nu\tau}\mathrm{e}^{3\lambda\tau}[a\delta_{\alpha,u_y} X_{u_x,k}(\mathrm{e}^{\lambda\tau}\Lambda_{ij}(-\tau)(v_j' - \delta u_j)) \\ -Y_{\alpha,k}(\mathrm{e}^{\lambda\tau}\Lambda_{ij}(-\tau)(v_j' - \delta u_j))]. \end{aligned} \tag{E.18}$$

APPENDIX F
TRANSPORT COEFFICIENTS

In this appendix, the transport coefficients defined in Eqs.(4.54) and (4.55) are calculated by using the solution to Eq.(4.47). First, the coefficients from momentum flux are considered,

$$\gamma_{lm}^{ij} = -\int d\mathbf{v}' m c_i c_j X_{u_l,m}, \tag{F.1}$$

where $\mathbf{c} = \mathbf{v}' - \delta\mathbf{u}$. As an example, the γ_{xy}^{xy} is analyzed. Since the γ_{xy}^{xy} is defined with $X_{u_x,y}$, the equation for $X_{u_x,y}$ is considered to solve

$$\left(\frac{\partial^{(0)}}{\partial t} - L(v',a) + \lambda\,\delta u_i \frac{\partial}{\partial v_i'} + \nu\right) X_{u_x,y} = -Y_{u_x,y}, \tag{F.2}$$

where the operator L is defined in (4.17). Substitution of the solution, $X_{u_x,y}$ (E.18) into the definition of γ_{xy}^{xy}, (F.1) gives

$$\gamma_{xy}^{xy} = -\int d\mathbf{v}'\, m c_x c_y \int_0^\infty dt\, \mathrm{e}^{-\nu t}\mathrm{e}^{3\lambda t} Y_{u_x,y}(\mathrm{e}^{\lambda t}\Lambda_{ij}(-t)c_j). \tag{F.3}$$

The γ_{xy}^{xy} can be calculated with couple of change of variables on velocity variables. First $\mathbf{v}' \to \mathbf{v}' + \delta\mathbf{u}$ and then $v_i' \to \mathrm{e}^{-\lambda t} v_i'$, and finally do $v_i' \to \Lambda_{ij}(t) v_j'$. Then γ_{xy}^{xy} is

$$\gamma_{xy}^{xy} = -\int_0^\infty dt\, \mathrm{e}^{-(\nu+2\lambda)t} m \int d\mathbf{v}\, (v_x - a t v_y) v_y$$

$$\times \left[-\frac{2}{3nk_B} \frac{\partial f^{(0)}}{\partial T} (t_{xy}^{(0)} + a_{lm}\gamma_{xy}^{lm}) + \frac{\partial f^{(0)}}{\partial \delta u_x} v_y \right] \tag{F.4}$$

$$= (t_{xy}^{(0)} + a\gamma_{xy}^{xy}) \left(\frac{2\nu a}{(2\lambda+\nu)^3} - \frac{10\nu a}{3(2\lambda+\nu)^3} \right) - \frac{\nu}{(2\lambda+\nu)^2} p. \tag{F.5}$$

Use of the result of $t_{xy}^{(0)}$ in (4.44b) and the relation of λ and shear rate a (4.22) gives the final value of the γ_{xy}^{xy},

$$\gamma_{xy}^{xy} = \frac{\nu(2\lambda-\nu)}{(2\lambda+\nu)^2(6\lambda+\nu)} p. \tag{F.6}$$

The same method is used for all the transport coefficients and they are as follows:

$$\gamma_{xx}^{xy}/p = \frac{2\,a\,\nu\,(\nu^2 - 18\,\nu\,\lambda - 72\,\lambda^2)}{3\,(\nu+2\,\lambda)^3\,(\nu+6\,\lambda)^2} \tag{F.7}$$

$$\gamma_{xy}^{xy}/p = \frac{\nu\,(-\nu+2\,\lambda)}{(\nu+2\,\lambda)^2\,(\nu+6\,\lambda)} \tag{F.8}$$

$$\gamma_{xz}^{xy}/p = 0 \tag{F.9}$$

$$\begin{aligned} \gamma_{yx}^{xy}/p = &-(\nu^6 + 28\,\nu^5\,\lambda + 417\,\nu^4\,\lambda^2 + 3087\,\nu^3\,\lambda^3 + 11622\,\nu^2\,\lambda^4 \\ &+21420\,\nu\,\lambda^5 + 15336\,\lambda^6)/((\nu+2\,\lambda)^3\,(\nu+3\,\lambda)^2\,(\nu+6\,\lambda)^2) \end{aligned} \tag{F.10}$$

$$\gamma_{yy}^{xy}/p = \frac{a\,\nu\,(5\,\nu^4 + 76\,\nu^3\,\lambda + 408\,\nu^2\,\lambda^2 + 912\,\nu\,\lambda^3 + 720\,\lambda^4)}{3\,(\nu+2\,\lambda)^5\,(\nu+3\,\lambda)\,(\nu+6\,\lambda)} \tag{F.11}$$

$$\gamma_{yz}^{xy}/p = 0 \tag{F.12}$$

$$\gamma_{zx}^{xy}/p = \gamma_{zy}^{xy}/p = 0 \tag{F.13}$$

$$\gamma_{zz}^{xy}/p = \frac{2a\,\lambda\,(6\lambda - 5\nu)}{(2\lambda+\nu)^2(6\lambda+\nu)^2} \tag{F.14}$$

$$\begin{aligned}\gamma_{xx}^{xx}/p = {} & (5\,\nu^8 + 119\,\nu^7\,\lambda + 1107\,\nu^6\,\lambda^2 + 2361\,\nu^5\,\lambda^3 - 26388\,\nu^4\,\lambda^4 \\ & -192096\,\nu^3\,\lambda^5 - 512784\,\nu^2\,\lambda^6 - 597456\,\nu\,\lambda^7 - 233280\,\lambda^8)/ \\ & (3\,\nu\,(\nu+2\,\lambda)^3\,(\nu+3\,\lambda)^3\,(\nu+6\,\lambda)^2)\end{aligned} \tag{F.15}$$

$$\gamma_{xy}^{xx}/p = \frac{4\,a\,(2\,\nu^5 + 26\,\nu^4\,\lambda + 166\,\nu^3\,\lambda^2 + 549\,\nu^2\,\lambda^3 + 852\,\nu\,\lambda^4 + 468\,\lambda^5)}{3\,(\nu+2\,\lambda)^4\,(\nu+3\,\lambda)^2\,(\nu+6\,\lambda)} \tag{F.16}$$

$$\gamma_{xz}^{xx}/p = 0 \tag{F.17}$$

$$\begin{aligned}\gamma_{yx}^{xx}/p = {} & (a(33\nu^{10} + 1084\nu^9\lambda + 15968\nu^8\lambda^2 + 115260\nu^7\lambda^3 \\ & +345843\nu^6\lambda^4 - 431136\nu^5\lambda^5 - 6653448\nu^4\lambda^6 - 21439728\nu^3\lambda 67 \\ & -32523120\nu^2\lambda^8 - 22243912\nu\lambda^9 - 4199040\lambda^{10})) / \\ & (9\nu(2\lambda+\nu)^5(3\lambda+\nu)^4(6\lambda+\nu)^2)\end{aligned} \tag{F.18}$$

$$\begin{aligned}\gamma_{yy}^{xx}/p = {} & (2\nu^6 + 15\nu^5\lambda - 16\nu^4\lambda^2 - 135\nu^3\lambda^3 + 222\nu^2\lambda^4 \\ & +252\nu\lambda^5 - 1368\lambda^6)\,/(3\nu(2\lambda+\nu)^4(3\lambda+\nu)^2)\end{aligned} \tag{F.19}$$

$$\gamma_{yz}^{xx}/p = 0 \tag{F.20}$$

$$\gamma_{5x}^{xx}/p = \gamma_{5y}^{xx}/p = 0 \tag{F.21}$$

$$\begin{aligned}\gamma_{zz}^{xx}/p = &(2(\nu^7 + 87\nu^6\lambda + 1521\nu^5\lambda^2 + 10497\nu^4\lambda^3 + 34344\nu^4\lambda^4 \\ &+57528\nu^2\lambda^5 \\ &+56592\nu\lambda^6 + 37584\lambda^7))\,/ \\ &(3\nu(2\lambda+\nu)^3(3\lambda+\nu)^2(6\lambda+\nu)^2)\end{aligned} \tag{F.22}$$

$$\gamma_{xx}^{yy}/p = \frac{2\,(\nu^3 + 24\,\nu^2\,\lambda + 72\,\nu\,\lambda^2)}{3\,(\nu+2\,\lambda)^2\,(\nu+6\,\lambda)^2} \tag{F.23}$$

$$\gamma_{xy}^{yy}/p = \frac{-4\,a\,\nu^2}{3\,(\nu+2\,\lambda)^3\,(\nu+6\,\lambda)} \tag{F.24}$$

$$\gamma_{xz}^{yy}/p = 0 \tag{F.25}$$

$$\begin{aligned}\gamma_{yx}^{yy}/p = &(2\,a\,\nu\,(2\,\nu^6 + 48\,\nu^5\,\lambda + 278\,\nu^4\,\lambda^2 + 3\,\nu^3\,\lambda^3 \\ &-4422\,\nu^2\,\lambda^4 - 12996\,\nu\,\lambda^5 - 11448\,\lambda^6))/ \\ &(3\,(\nu+2\,\lambda)^5\,(\nu+3\,\lambda)^2\,(\nu+6\,\lambda)^2)\end{aligned} \tag{F.26}$$

$$\gamma_{yy}^{yy}/p = \frac{2\,\nu\,(-2\,\nu^3 - 11\,\nu^2\,\lambda - 6\,\nu\,\lambda^2 + 24\,\lambda^3)}{3\,(\nu+2\,\lambda)^4\,(\nu+3\,\lambda)} \tag{F.27}$$

$$\gamma_{yz}^{yy}/p = 0 \tag{F.28}$$

$$\gamma_{zx}^{yy}/p = \gamma_{zy}^{yy}/p = 0 \tag{F.29}$$

$$\gamma_{zz}^{yy}/p = \frac{2(\nu^5 + 12\nu^4\lambda - 36\nu^3\lambda^2 - 582\nu^2\lambda^3 - 1512\nu\lambda^4 - 1080\lambda^5)}{3(2\lambda+\nu)^3(3\lambda+\nu)(6\lambda+\nu)^2} \tag{F.30}$$

$$\gamma_{xx}^{zz}/p = \frac{2\nu(\nu^2 + 24\lambda\nu + 72\lambda^2)}{3(2\lambda+\nu)^2(6\lambda+\nu)^2} \tag{F.31}$$

$$\gamma_{xy}^{zz}/p = -\frac{4\nu^2 a}{3(2\lambda+\nu)^3(6\lambda+\nu)} \tag{F.32}$$

$$\gamma_{xz}^{zz}/p = 0 \tag{F.33}$$

$$\begin{aligned}\gamma_{yx}^{zz}/p = {} & (2a(-\nu^7 - 5\nu^6\lambda - 41\nu^5\lambda^2 - 573\nu^4\lambda^3 - 2982\nu^3\lambda^4 \\ & -5508\nu^2\lambda^5 - 648\nu\lambda^6 + 5184\lambda^7))/ \\ & (3(2\lambda+\nu)^5(3\lambda+\nu)^2(6\lambda+\nu)^2)\end{aligned} \tag{F.34}$$

$$\gamma_{yy}^{zz}/p = \frac{2\nu(6\lambda+\nu)(\nu^2 + 14\lambda\nu + 30\lambda^2)}{3(2\lambda+\nu)^4(3\lambda+\nu)} \tag{F.35}$$

$$\gamma_{yz}^{zz}/p = 0 \tag{F.36}$$

$$\gamma_{zx}^{zz}/p = \gamma_{zy}^{zz}/p = 0 \tag{F.37}$$

$$\gamma_{zz}^{zz}/p = \frac{4\nu(-\nu^4 - 5a\nu\lambda - 14\lambda\nu^3 + 6a\lambda^2 - 72\lambda^2\nu^2 - 168\nu\lambda^3 - 144\lambda^4)}{3(2\lambda+\nu)^4(6\lambda+\nu)^2} \tag{F.38}$$

$$\gamma_{xx}^{xz}/p = \gamma_{xy}^{xz}/p = 0 \tag{F.39}$$

$$\gamma_{xz}^{xz}/p = -\frac{\nu}{(2\lambda+\nu)^2} \tag{F.40}$$

$$\gamma_{yx}^{xz}/p = \gamma_{yy}^{xz}/p = \gamma_{yz}^{xz}/p = 0 \tag{F.41}$$

$$\begin{aligned}\gamma_{zz}^{xz}/p = &-(\nu^6 + 7\lambda\nu^5 + 48\nu^4\lambda^2 + 216\nu^3\lambda^3 + 447\nu^2\lambda^4 \\ &+399\nu\lambda^5 + 144\lambda^6)/(\nu(\lambda+\nu)(2\lambda+\nu)^2(3\lambda+\nu^3))\end{aligned} \tag{F.42}$$

$$\gamma_{zy}^{xz}/p = \frac{2\nu a(\nu^2 + 5\lambda\nu + 7\lambda^2)}{(2\lambda+\nu)^4(3\lambda+\nu)} \tag{F.43}$$

$$\gamma_{zz}^{xz}/p = 0 \tag{F.44}$$

$$\gamma_{xx}^{yz}/p = \gamma_{xy}^{yz}/p = \gamma_{xz}^{yz}/p = 0 \tag{F.45}$$

$$\gamma_{yx}^{yz}/p = \gamma_{yy}^{yz}/p = 0 \tag{F.46}$$

$$\gamma_{yz}^{yz}/p = -\frac{\nu}{(2\lambda+\nu)^2} \tag{F.47}$$

$$\gamma_{zx}^{yz}/p = \frac{a(\nu^2+5\lambda\nu+8\lambda^2)}{(2\lambda+\nu)^3(3\lambda+\nu)} \tag{F.48}$$

$$\gamma_{zy}^{yz}/p = \frac{2\lambda}{(2\lambda+\nu)^2} \tag{F.49}$$

$$\gamma_{zz}^{yz}/p = 0 \tag{F.50}$$

$$\begin{aligned}\frac{m}{nk_B^2T}\xi_{T,y}^{y} = &(-(5\,\nu^8+186\,\nu^7\,\lambda+2215\,\nu^6\,\lambda^2+13480\,\nu^5\,\lambda^3+49144\,\nu^4\,\lambda^4\\ &+112992\,\nu^3\,\lambda^5+159552\,\nu^2\,\lambda^6+122688\,\nu\,\lambda^7+36864\,\lambda^8))/\\ &(2\,\nu\,(\nu+2\,\lambda)^2\,(\nu+3\,\lambda)^3\,(\nu+4\,\lambda)^3)\end{aligned} \tag{F.51}$$

$$\begin{aligned}\frac{m}{nk_B^2T}\xi_{T,x}^{y} = &(a\,(9\,\nu^9+108\,\nu^8\,\lambda-641\,\nu^7\,\lambda^2-16802\,\nu^6\,\lambda^3-116528\,\nu^5\,\lambda^4\\ &-419184\,\nu^4\,\lambda^5-879808\,\nu^3\,\lambda^6\\ &-1096896\,\nu^2\,\lambda^7-772992\,\nu\,\lambda^8-248832\,\lambda^9))/\\ &(2\,\nu\,(\nu+2\,\lambda)^3\,(\nu+3\,\lambda)^3\,(\nu+4\,\lambda)^4)\end{aligned} \tag{F.52}$$

$$\begin{aligned}\frac{m}{nk_B^2T}\xi_{T,x}^{x} = &-(5\,\nu^{13}+a\,\nu^{11}\,\lambda+278\,\nu^{12}\,\lambda+26\,a\,\nu^{10}\,\lambda^2+7865\,\nu^{11}\,\lambda^2\\ &+289\,a\,\nu^9\,\lambda^3+111924\,\nu^{10}\,\lambda^3+1780\,a\,\nu^8\,\lambda^4+926254\,\nu^9\,\lambda^4\\ &+6560\,a\,\nu^7\,\lambda^5+4918220\,\nu^8\,\lambda^5+14464\,a\,\nu^6\,\lambda^6+17797024\,\nu^7\,\lambda^6\\ &+17664\,a\,\nu^5\,\lambda^7+45657536\,\nu^6\,\lambda^7+9216\,a\,\nu^4\,\lambda^8+85373952\,\nu^5\,\lambda^8\end{aligned}$$

$$+118065024\,\nu^4\,\lambda^9 + 119017728\,\nu^3\,\lambda^{10} + 81077760\,\nu^2\,\lambda^{11}$$
$$+30633984\,\nu\,\lambda^{12} + 3538944\,\lambda^{13})/$$
$$(2\,\nu^2\,(\nu+2\,\lambda)^3\,(\nu+3\,\lambda)^4\,(\nu+4\,\lambda)^5) \tag{F.53}$$

$$\frac{m}{nk_B^2T}\xi^x_{T,y} = (14\,a\,\nu^{10} + 317\,a\,\nu^9\,\lambda + \nu^{10}\,\lambda + 3078\,a\,\nu^8\,\lambda^2 + 24\,\nu^9\,\lambda^2 + 17835\,a\,\nu^7\,\lambda^3$$
$$+245\,\nu^8\,\lambda^3 + 75678\,a\,\nu^6\,\lambda^4 + 1378\,\nu^7\,\lambda^4 + 268688\,a\,\nu^5\,\lambda^5 + 4608\,\nu^6\,\lambda^5$$
$$+776528\,a\,\nu^4\,\lambda^6 + 9152\,\nu^5\,\lambda^6 + 1594080\,a\,\nu^3\,\lambda^7 + 9984\,\nu^4\,\lambda^7$$
$$+2017152\,a\,\nu^2\,\lambda^8 + 4608\,\nu^3\,\lambda^8 + 1323648\,a\,\nu\,\lambda^9 + 304128\,a\,\lambda^{10})/$$
$$(2\,\nu\,(\nu+2\,\lambda)^3\,(\nu+3\,\lambda)^4\,(\nu+4\,\lambda)^4) \tag{F.54}$$

$$\frac{m}{nk_B^2T}\xi^z_{T,z} = (-5\nu^7 - 42\nu^6\lambda + 203\nu^5\lambda^2 + 3566\nu^4\lambda^3 + 16364\nu^3\lambda^4$$
$$+35376\nu^2\lambda^5 + 37536\nu\lambda^6 + 16128\lambda^7)/$$
$$(2\nu(2\lambda+\nu)(3\lambda+\nu)^3(4\lambda+\nu)^3) \tag{F.55}$$

$$\frac{m}{k_B^2T^2}\xi^y_{n,x} = (a\,(-\nu^{13} - 401\,\nu^{12}\,\lambda - 10705\,\nu^{11}\,\lambda^2 - 135383\,\nu^{10}\,\lambda^3 - 1053900\,\nu^9\,\lambda^4$$
$$-5568818\,\nu^8\,\lambda^5 - 20669200\,\nu^7\,\lambda^6 - 53491128\,\nu^6\,\lambda^7 - 91320528\,\nu^5\,\lambda^8$$
$$-85889792\,\nu^4\,\lambda^9 - 4286976\,\nu^3\,\lambda^{10} + 86142080\,\nu^2\,\lambda^{11} + 86512896\,\nu\,\lambda^{12}$$
$$+29505024\,\lambda^{13} + \frac{2488320\,\lambda^{14}}{\nu}))/$$
$$((\nu+2\,\lambda)^4\,(\nu+3\,\lambda)^5\,(\nu+4\,\lambda)^5\,(\nu+6\,\lambda)) \tag{F.56}$$

$$\frac{m}{k_B^2T^2}\xi^y_{n,y} = (\lambda\,(29\,\nu^{11} + 739\,\nu^{10}\,\lambda + 9717\,\nu^9\,\lambda^2 + 78521\,\nu^8\,\lambda^3$$
$$+383576\,\nu^7\,\lambda^4 + 994366\,\nu^8\,\lambda^5 + 404636\,\nu^5\,\lambda^6 - 5601664\,\nu^4\,\lambda^7$$
$$-18060048\,\nu^3\,\lambda^8 - 26083104\,\nu^2\,\lambda^9 - 18698112\,\nu\,\lambda^{10} - 5336064\,\lambda^{11}))/$$

$$(\nu\,(\nu+2\,\lambda)^2\,(\nu+3\,\lambda)^5\,(\nu+4\,\lambda)^4\,(\nu+6\,\lambda)) \tag{F.57}$$

$$\begin{aligned}\frac{m}{k_B^2T^2}\xi^z_{n,z} = (&2\lambda(4\nu^1 1 + 113\nu^1 0\lambda + 1218\nu^9\lambda^2 + 6285\nu^8\lambda^3 + 13216\nu^7\lambda^4\\ &-17468\nu^6\lambda^5 - 170096\nu^5\lambda^6 - 460452\nu^4\lambda^7 - 848880\nu^3\lambda^8\\ &-1461168\nu^2\lambda^9 - 1912896\nu\lambda^1 0 - 1133568\lambda^1 1))/\\ &(\nu(2\lambda+\nu)^2(3\lambda+\nu)^5(4\lambda+\nu)^4(6\lambda+\nu))\end{aligned} \tag{F.58}$$

APPENDIX G
THE HYDRODYNAMIC MODES

In this appendix, the calculation of the hydrodynamic modes, $\delta\tilde{y}_\alpha(t)$, for special case $a^* = 0.5$ and $k^* = 0.1$ is done from Eq.(5.25) to compare the behavior of the instability with the results from simulations. The simulations were performed using a thermostat with constant λ, rather than $\lambda = \lambda(n(\mathbf{r},t), T(\mathbf{r},t))$ as considered here. To account for this, the linearized equation for the temperature in (5.8) has two additional terms that couple the temperature to itself and the density. These arise since there is no complete cancelation of viscous heating to lowest order in the spatial gradients. For convenience, we use dimensionless variables; i.e.,

$$z^* = z/\nu, \quad k^* = kv_0/\nu = \sqrt{\frac{2k_BT}{m}}k/\nu, \tag{G.1}$$

$$\lambda^* = \lambda/\nu, \quad a^* = a/\nu. \tag{G.2}$$

From now on, we considered only two dimension case (x, y dimension), since z-component is not coupled to other components so it gives a result (5.57). Also we drop the $*$ sign from now on. Then the determinant of the matrix K becomes a fourth order polynomial function for z,

$$\begin{aligned}\det[K_{\alpha\beta}(k=0.1,z)] = {} & 2.04302\,10^{-6} + 0.000666015\,z + 0.00891949\,z^2 \\ & +0.0190414\,z^3 + z^4,\end{aligned} \tag{G.3}$$

and the solutions for $\det(K) = 0$ are

$$z_1 = -0.0569012, \quad z_2 = -0.00320425, \quad z_3 = 0.020532 - i0.103845, \quad z_4 = z_3^*. \tag{G.4}$$

The dynamics of $\delta\widetilde{y}_\alpha(t)$ in (5.20) is determined from these poles. The first two poles are negative, so their modes are stable, whereas the complex conjugate pair z_3 and z_4 represents unstable modes since the real parts of the poles are positive. It is easy to see this situation if we write down the expression of $\delta y_\alpha(t)$ with these poles. The Eq.(5.25) can be written

$$\widehat{\delta y}_\alpha(k = 0.1, z) = \frac{N_{\alpha\beta}(k = 0.1, z)}{(z - z_1)(z - z_2)(z - z_3)(z - z_4)} \delta\widetilde{y}_\beta(k = 0.1, t = 0), \tag{G.5}$$

where $K^{-1}_{\alpha\beta} = \frac{N_{\alpha\beta}}{\det(K)}$, and the inverse Laplace transformation of $\widehat{\delta y}_\alpha$ gives complete expression of $\delta\widetilde{y}_\alpha(t)$ in terms of initial conditions,

$$\delta\widetilde{y}_\alpha(t) = \sum_{i=1}^{4} \frac{e^{z_i t}}{\prod_{j\neq i}(z_i - z_j)} \sum_{\beta=1}^{4} N_{\alpha\beta}(z = z_i)\delta\widetilde{y}_\beta(t = 0). \tag{G.6}$$

It is clearly seen that z_3 and z_4 are responsible for instability. The matrix elements of $N_{\alpha\beta}$ in Eq.(G.6) are

$$N_{11} = 0.000936892 + 0.00366708\, z + 0.0190414\, z^2 + z^3, \tag{G.7a}$$

$$N_{12} = -0.0000114814 - 0.00361146\, z, \tag{G.7b}$$

$$N_{13} = 0.000131178\, i - 0.00011728\, i\, z, \tag{G.7c}$$

$$N_{14} = 0.0000607019\, i + 0.0010161\, i\, z + 0.0707107\, i\, z^2, \tag{G.7d}$$

$$N_{21} = -0.00129203 - 0.00625125\,z - 0.0962409\,z^2, \tag{G.7e}$$

$$N_{22} = 0.0000140618 + 0.00443992\,z + 0.00711708\,z^2 + z^3, \tag{G.7f}$$

$$N_{23} = -0.000181528\,i - 0.000287276\,i\,z - 0.0367099\,i\,z^2, \tag{G.7g}$$

$$N_{24} = -0.0000435735\,i + 0.0116013\,i\,z + 0.0698092\,i\,z^2, \tag{G.7h}$$

$$N_{31} = 0.00209147\,i - 0.0348971\,i\,z - 0.0103748\,i\,z^2, \tag{G.7i}$$

$$N_{32} = -0.000081186\,i - 0.0254766\,i\,z - 0.0225905\,i\,z^2, \tag{G.7j}$$

$$N_{33} = -0.000284938 + 0.00887352\,z + 0.0165958\,z^2 + z^3, \tag{G.7k}$$

$$N_{34} = -0.000144986 - 0.00361283\,z - 0.496755\,z^2, \tag{G.7l}$$

$$N_{41} = 0.0000288927\,i - 0.00383077\,i\,z + 0.0742802\,i\,z^2, \tag{G.7m}$$

$$N_{42} = 0.000162372\,i\,z + 0.0510737\,i\,z^2, \tag{G.7n}$$

$$N_{43} = ,0.00185513\,z - 0.00165859\,z^2, \tag{G.7o}$$

$$N_{44} = 0.000858455\,z + 0.0143699\,z^2 + z^3. \tag{G.7p}$$

Now we need to determine the initial conditions for $\delta\tilde{y}_\alpha(t)$ in order to see the dynamics of the hydrodynamic modes with instability. We chose the initial condition such that $\delta\tilde{u}_y(t)$ is dominated mostly by unstable modes. The results are shown in section 5.2 and the figure 5.2 shows the results for $\delta\tilde{u}_x(t)$ and $\delta\tilde{u}_y(t)$ as a function of time and they are in good agreement with the results from simulations.

APPENDIX H
CORRELATION FUNCTIONS

The matrix H^{ij} is defined in (6.8). The elements of $H^{ij} = H^{ji}$ and are given by

$$H^{11} = -5x^2 \frac{4\lambda}{2\lambda + \nu}, \tag{H.1}$$

$$H^{12} = -H^{11}, \tag{H.2}$$

$$H^{13} = \frac{i}{2}\sqrt{5}x \frac{\nu a}{(2\lambda + \nu)^2}, \tag{H.3}$$

$$H^{14} = -H^{13}, \tag{H.4}$$

$$H^{22} = \frac{3}{5}Q + H^{11}, \tag{H.5}$$

$$H^{23} = \sqrt{\frac{3}{50}}Q - H^{13}, \tag{H.6}$$

$$H^{24} = \sqrt{\frac{3}{50}}Q + H^{13}, \tag{H.7}$$

$$H^{33} = \frac{1}{10}Q - \frac{\lambda}{2(2\lambda + \nu)}, \tag{H.8}$$

$$H^{34} = \frac{1}{10}Q + \frac{\lambda}{2(2\lambda + \nu)}, \tag{H.9}$$

$$H^{44} = H^{33}, \tag{H.10}$$

where $Q \equiv \frac{1}{6}\left[-\frac{60\lambda}{4\lambda+\nu} + \frac{28\nu a^2}{(4\lambda+\nu)^3} + \frac{72\nu a^4}{(4\lambda+\nu)^5}\right]$.

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